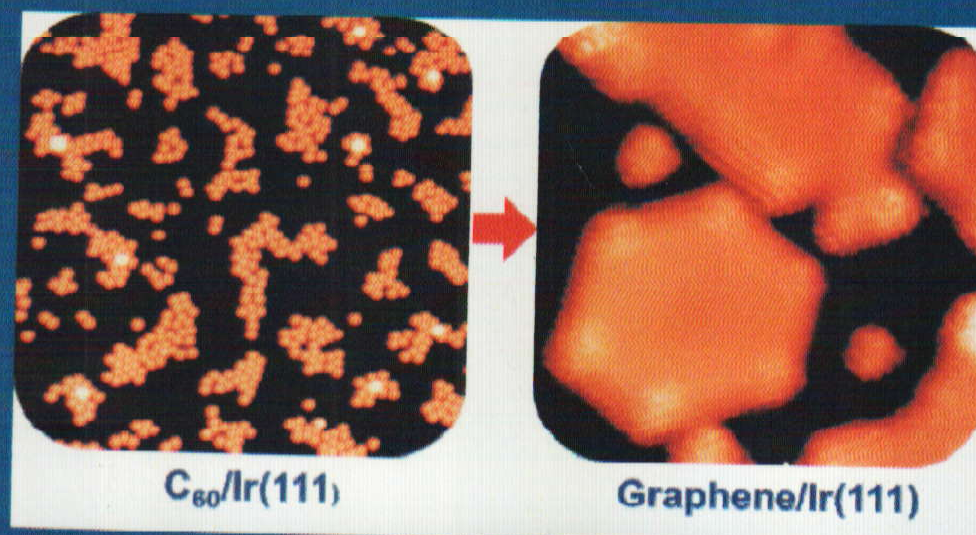
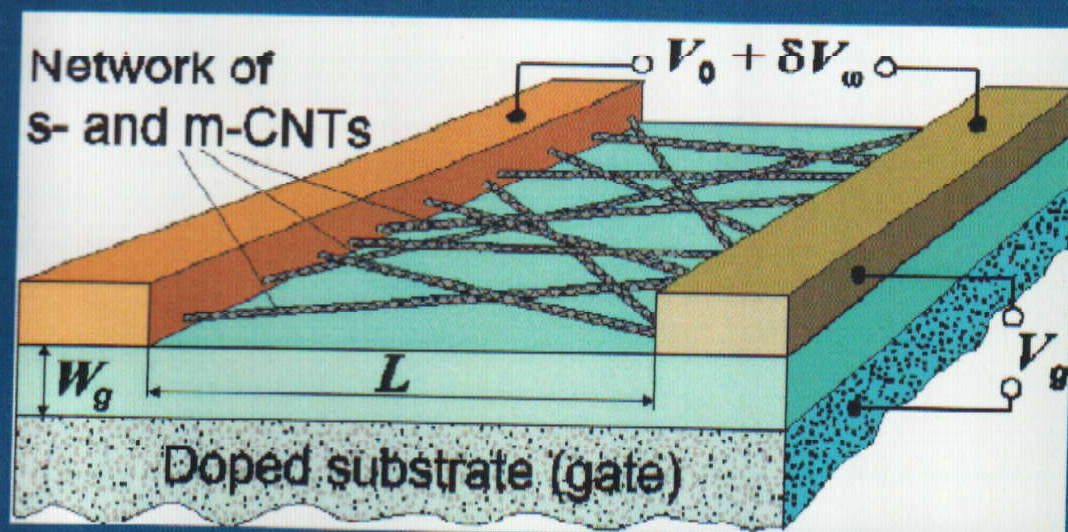
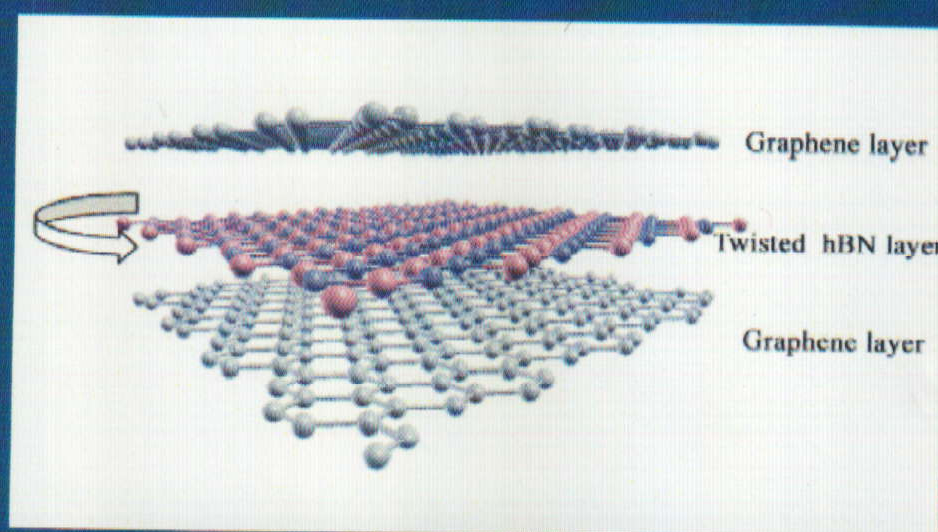
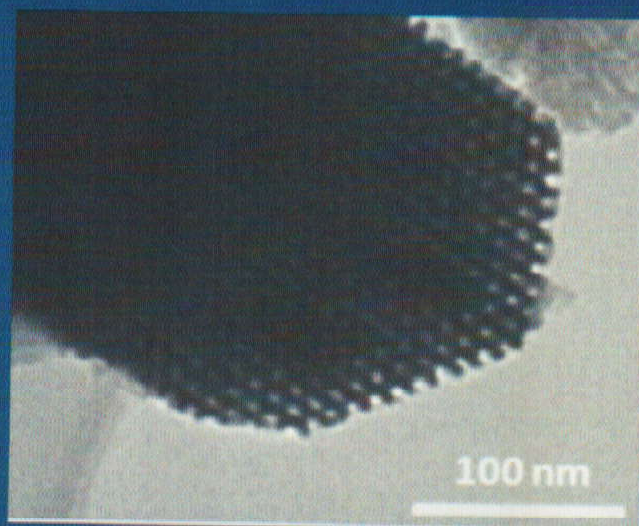


# EMN MEETING

EMN Meeting on Carbon Nanostructures 2016  
Energy Materials Nanotechnology  
March 27-31, 2016, Hawaii, USA

## PROGRAM & ABSTRACT





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### Registration Desk Hours

The EMN Meeting on Carbon Nanostructures registration desk, located in The DoubleTree by Hilton Hotel Aina-Waikiki Beach, will be open during the following hours:



## General Information

The 2016 EMN Meeting on Carbon Nanostructures will take place at The DoubleTree by Hilton Hotel Alana – Waikiki Beach, Hawaii, USA. The conference will be held from March 27 to 31, 2016.

Workshops on selected focus topics will include invited and contributed oral presentations from Monday to Wednesday and the poster session will be presented on the afternoon of Tuesday (March 29).

### Registration Desk Hours

The EMN Meeting on Carbon Nanostructures registration desk, located in The DoubleTree by Hilton Hotel Alana-Waikiki Beach, will be open during the following hours:

March 27.....	14:00pm -18:00pm
March 28.....	7:00am -18:00pm
March 29.....	7:00am -18:00pm
March 30.....	7:00am -18:00pm



## **EMN Meeting on Carbon Nanostructures Committee**

### **International Advisory Committee**

**Bharat Bhushan**, Ohio State University, USA

**Vancso G. Julius**, University of Twente, Netherlands

### **International Program Committee**

**Jiming Bao**, University of Houston, USA

**Bingqing Wei**, University of Delaware, USA

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**Alan B. Dalton**, University of Surrey, United Kingdom

**Zhiming Wang**, University of Electronic Science and Technology of China, China

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**Mehrdad Nejhad**, University of Hawaii at Manoa, USA

### **General Chair**

**Zhiming Wang**, Institute of Fundamental and Frontier Sciences, UESTC, China



## EMN Meeting on Carbon Nanostructures

## Program-at-a-Glance

Monday, March 28	
Room A(Pikake)	
Nanotubes Applications I	8:25-10:05 AM
Graphene-General I	10:25-12:05 PM
Tuesday, March 29	
Room B(Naupake I&II)	
Theory, Simulations and Modeling of Nanotubes	8:00-10:05 AM
Synthesis and Assembly of Nanotubes I	10:25-12:05 PM
Nanotubes-General I	13:20-15:00 PM
Poster Session	15:00-15:50 PM
Graphene-General II	15:50-17:55 PM
Room C(Oheho)	
Electronic properties of graphene I	8:00-10:05 AM
Graphene Application	10:25-12:05 PM
Wednesday, March 30	
Room B(Naupake I&II)	
Synthesis and Assembly of Nanotubes II	8:25-10:05 AM
Fundamental properties of Nanotubes	10:25-12:05 PM
Nanotubes-General II	13:35-18:00 PM
Room C(Ohelo)	
Nanotubes Applications II	8:00-10:05 AM
Electronic properties of Graphene II	10:25-12:05 PM



Sunday March 27		
14:00-18:00 PM	Onsite Registration & Sign up	
Monday Morning March 28 Room A(Pikake)		
8:20-8:25 AM	Opening Ceremony	
Session: Nanotubes Applications I		Chair: Moon Kim
8:25-8:50 AM	A01: Energy storage using carbon-based nanoporous material structures	<b>Jisoon Ihm</b> Scoul National University, Korea
8:50-9:15 AM	A02: Production of Carbon Nanotubes from Graphite via Molten Salt Electrochemistry and their Application in Energy Devices	<b>Carsten Schwandt</b> University of Nizwa, Oman
9:15-9:40 AM	A03: 3-D nickel-metal layered double hydroxide/CNT nano-architecture composites for high power energy storage application	<b>Zexiang Chen</b> University of Electronic Science and Technology of China, China
9:40-10:05 AM	A04: Nanocomposite Fabric Sensors for Human Performance Monitoring	<b>Kenneth J. Loh</b> University of California San Diego, USA
10:05-10:25 AM	Session Break	
Session: Graphene-General I		Chair: Jisoon Ihm
10:25-10:50 AM	A05: Probing carbon nanostructures for nanoelectronics down to atomic scale	<b>Moon Kim</b> University of Texas at Dallas, USA
10:50-11:15 AM	A06: Chemically engineered graphene like carbon layers and nanotubes	<b>Jacek A. Majewski</b> University of Warsaw, Poland
11:15-11:40 AM	A07: Dynamic TEM observation of the formation of graphene and carbon nanotubes	<b>Masaki Tanemura</b> Nagoya Institute of Technology, Japan
11:40-12:05 PM	A08: Controlling the band structure of black phosphorus	<b>Keun Su Kim</b> Pohang University of Science and Technology, Korea
18:00 PM	Dinner Social	



**Tuesday Morning March 29**  
**Room B(Naupake I&II)**

**Session: Theory, Simulations and Modeling of Nanotubes**

**Chair: Bingqing Wei**

8:00-8:25 AM	B01: Density functional theory calculation for transport property of carbon nanostructures	<b>Tomoya Ono</b> University of Tsukuba, Japan
8:25-8:50 AM	B02: Detection of terahertz radiation by two-dimensional plasmons in lateral carbon nanotube networks	<b>Victor Ryzhii</b> Tohoku University, Japan
8:50-9:15 AM	B03: Mechanics modeling on the mechanical and electrical properties of carbon nanotube (CNT)-polymer composites	<b>Liyang Jiang</b> University of Western Ontario, Canada
9:15-9:40 AM	B04: Simulation Studies of Nanotube Formation by Polymer Adsorption at a Nanowire	<b>Michael Bachmann</b> University of Georgia, USA
9:40-10:05 AM	B05: Atomistic modeling of buckling behavior of pressurized nanotubes	<b>Yoshitaka Umeno</b> University of Tokyo, Japan
10:05-10:25 AM	Session Break	
<b>Session: Synthesis and Assembly of Nanotubes I</b>		<b>Chair: Tomoya Ono</b>
10:25-10:50 AM	B06: Tailoring Carbon Nanotube Assembly for Energy Storage Applications	<b>Bingqing Wei</b> University of Delaware, USA
10:50-11:15 AM	B07: Investigating Growth Termination Mechanism of Carbon Nanotube Arrays Using Transmission Electron Microscopy Approach	<b>Seung Min Kim</b> Korea Institute of Science and Technology, Korea
11:15-11:40 AM	B08: Micro Indentation of densely aligned CNTs film grown on SiC substrate	<b>Hatsuhiko Usami</b> Meijo University, Japan
11:40-12:05 PM	B09: Biologically assembled conductive nanomesh of single-walled carbon nanotubes for wearable biosensors and devices	<b>Hyunjung Yi</b> Korea Institute of Science and Technology, Korea
12:05-13:20 PM	Lunch Break	



Tuesday Morning March 29 Room C(Oheho)		
Session: Graphene Application		Chair: Roger Lake
8:00-8:25 AM	C01: Graphene nanosystems and low-dimensional Chern-Simons topological insulators	<b>Eric Yang</b> Korea University, Korea
8:25-8:50 AM	C02: Graphene - Nano-electromechanical system switches and van der Waals (vdW) interaction controlled sensing of CO <sub>2</sub>	<b>Manoharan Muruganathan</b> Japan Advanced Institute of Science and Technology, Japan
8:50-9:15 AM	C03: Stretchable, Transparent Electrodes using hybrid structures of 1D-2D Nanomaterials for Wearable Electronics	<b>Jang-Ung Park</b> Ulsan National Institute of Science and Technology, Korea
9:15-9:40 AM	C04: Modified Epitaxial Graphene on SiC for Selective and Highly Sensitive Gas Sensors	<b>Jens Eriksson</b> Linköping University, Sweden
9:40-10:05 AM	C05: Applications of Nanotechnology in Fuel Energy and Propulsion	<b>Bruce Chehroudi</b> Advanced Technology Consultants, USA
10:05-10:25 AM	Session Break	
Session: Electronic properties of Graphene I		Chair: Eric Yang
10:25-10:50 AM	C06: Electron transport through graphene-BN-graphene heterostructures	<b>Roger Lake</b> University of California Riverside, USA
10:50-11:15 AM	C07: Edge configurational effect on band gaps in Graphene nanoribbons	<b>Rakesh Kumar</b> Indian Institute of Technology Ropar, India
11:15-11:40 AM	C08: Van der Waals stacks of few-layer h-AlN with graphene: an ab-initio study of structural, interaction and electronic properties	<b>Gueorgui K. Gueorguiev</b> Linköping University, Sweden
11:40-12:05 PM	C09: Scanning Tunneling Microscopy Studies of Hydrogen Desorption from Graphene and Transformation of C <sub>60</sub> into Graphene	<b>Li Gao</b> California State University Northridge, USA
12:05-13:20 PM	Lunch Break	



Tuesday Afternoon March 29 Room B(Naupake I&II)		
Session: Nanotubes-General I		Chair: Julia Zhao
13:20-13:45 PM	B10: Thermo/Piezo – Electric Power Scavenging Using Carbon Nanotube Composites	<b>David Carroll</b> Wake Forest University, USA
13:45-14:10 PM	B11: Megagauss Magneto-optical Survey of Exciton States in Single-wall Carbon Nanotubes	<b>Shojiro Takeyama</b> University of Tokyo, Japan
14:10-14:35 PM	B12: Carbon Capture using Waste Polymers Supported on SBA-15 silica and other Nanoporous Materials	<b>Humphrey Yiu</b> Heriot-Watt University, UK
14:35-15:00 PM	B13: Towards Realizing a SWCNT Industry from Fundamental Science	<b>Don Futaba</b> National Institute of Advanced Industrial Science and Technology, Japan
15:00-15:50 PM	Session Break & Poster Session	
	P01: Studies on the equivalent serial resistance of carbon supercapacitor	<b>Changping Yang</b> Hubei University, China
	P02: Partial Phase Coherence in Noise-Like Pulses Generated in Mode-Locked Laser Systems	<b>Yoonchan Jeong</b> Seoul National University, Korea
	P03: Continuous dispersion of carbon nanotubes with minimal loss and damage	<b>Hiroyuki Shirae</b> Waseda university, Japan
Session: Graphene-General II		Chair: David Carroll
15:50-16:15 PM	B14: Development of fluorescent graphene quantum dots for bioimaging	<b>Julia Zhao</b> University of North Dakota, USA
16:15-16:40 PM	B15: Anomalous enhancement of Seebeck coefficients for the graphene/h-BN composites	<b>Jun Nakamura</b> University of Electro-Communications, Japan
16:40-17:05 PM	B16: Quantum interference effects in graphene nanostructures	<b>Adam Rycerz</b> Jagiellonian University, Poland
17:05-17:30 PM	B17: In-situ Raman spectroscopy of graphene thin films containing palladium particles at the presence of hydrogen atoms	<b>Ali Moafi</b> Australian Microscopy and Microanalysis Research Facility, Australia
17:30-17:55 PM	B18: Ag Nanoparticles/ Graphene Oxide (GO)/ $\alpha$ -Bi <sub>2</sub> O <sub>3</sub> Hybrid Versatile Composites for Visible Light Photocatalysis and Chemical Catalysis	<b>Tirtha Som</b> Institute Nanospectroscopy and Energy Materials In Situ Laboratory, Germany
18:00 PM	Dinner Social	



Wednesday Morning March 30 Room B(Naupake I&II)		
Session: Synthesis and Assembly of Nanotubes II		Chair: Sookyung Moon
8:25-8:50 AM	B19: Self-assembled nanotube with enzymatic functionality	<b>Junqiu Liu</b> Jilin University, China
8:50-9:15 AM	B20: Self-assembled Films of Polyaniline and Carbon Nanotubes: their use as transparent electrodes and gas sensors	<b>Lucimara Stolz Roman</b> Federal University of Paraná, Brasil
9:15-9:40 AM	B21: Forming CNT-Guided Stereocomplex Networks in Polylactide-Based Nanocomposites	<b>Guozhang Wu</b> East China University of Science and Technology, China
9:40-10:05 AM	B22: Self-Assembly of Peptides into Nanotubes	<b>Seyda Bucak</b> Yeditepe University, Turkey
10:05-10:25 AM	Session Break	
Session: Fundamental properties of Nanotubes		Chair: Junqiu Liu
10:25-10:50 AM	B23: Enhanced Mechanical property of Aligned Carbon Nanotubes /Polymer composite	<b>Sookyung Moon</b> Japan Aerospace Exploration Agency, Japan
10:50-11:15 AM	B24: Thermo-mechanical properties of Carbon nanotubes and applications in thermal management	<b>Phan Ngoc Minh</b> Vietnam Academy of Science and Technology, Vietnam
11:15-11:40 AM	B25: Preparation and property of polyaniline nanocomposites containing TiO <sub>2</sub> nanoparticles and carbon nanotubes	<b>Noriyuki Kuramoto</b> Yamagata University, Japan
11:40-12:05 PM	B26: Nonlinear Mechanical Resonance of Cantilevered Carbon Nanotube with Electrostatic Excitation	<b>Sooil Lee</b> University of Seoul, Korea
12:05-13:20 PM	Lunch Break	



Wednesday Morning March 30 Room C(Ohelo)		
Session: Nanotubes Applications II		Chair: Jeffrey M. Mativetsky
8:00-8:25 AM	C10: Application of Nanotube/Nanotechnology in Structures and Renewable Energy Productions and Storage Devices	<b>Mehrdad Nejhad</b> University of Hawai'i at Manoa, USA
8:25-8:50 AM	C11: Analytical applications of carbon nanotubes based electrochemical sensors	<b>Anton Alexandru Ciucu</b> University of Bucharest, Romania
8:50-9:15 AM	C12: Carbon Nanotube for Cardiovascular Engineering Applications	<b>David A Stout</b> California State University, USA
9:15-9:40 AM	C13: Routes to carbon nanotube assembly and integration for applications	<b>Chris Papadopoulos</b> University of Victoria, Canada
9:40-10:05 AM	C14: Nanostructured Glass Fibers for Electro-Mechanical Response Sensor Applications in Glass Fiber Composites	<b>Michael Mueller</b> Leibniz Institute of Polymer Research Dresden, Germany
10:05-10:25 AM	Session Break	
Session: Electronic properties of Graphene II		Chair: Mehrdad Nejhad
10:20-10:50 AM	C15: Multiscale Patterning of Electrical Function in Graphene Oxide	<b>Jeffrey M. Mativetsky</b> State University of New York, USA
10:50-11:15 AM	C16: Graphene examined with ultraslow electrons	<b>Ludek Frank</b> Institute of Scientific Instruments, Academy of Sciences of the Czech Republic, Czech Republic
11:15-11:40 AM	C17: Computational Design of Graphene-Nanoribbon Field Effect Transistors	<b>Kengo Takashima</b> Tokyo University of Science, Japan
11:45-12:05 PM	C18: Functionalizing graphene via interface engineering	<b>Chan-Cuk Hwang</b> Pohang University of Science and Technology, Korea
12:05-13:35 PM	Lunch Break	



Wednesday Afternoon March 30 Room B(Naupake I&II)		
Session: Nanotubes-General II		Chair: Shadi Hasan
13:35-14:00 PM	B27: Stiffness and conformation dependent polymer wrapping of SWCNT	<b>Masanobu Naito</b> National Institute for Materials Science, Japan
14:00-14:25 PM	B28: Anisotropic Interaction of Ferromagnetic Nanoparticles Intercalated in Aligned Array of Carbon Nanotubes	<b>Serghej L. Prischepa</b> Belarus State University, Belarus
14:25-14:50 PM	B29: Production and reactivity of oxidation-resistant metallic nanoparticles on carbon nanotubes	<b>Hideki Tanaka</b> Faculty of Science and Engineering, Chuo University, Japan
14:50-15:15 PM	B30: Anodic Oxide Nanotubes for Energy Applications: Understanding Formation Mechanism and Defect Structures	<b>Krishnan Raja</b> University of Idaho, USA
15:15-15:30PM	Session Break	
15:30-15:55 PM	B31: Fabrication of CNT network and its application to GaN-based LEDs	<b>Tae Geun Kim</b> Korea University, Korea
15:55-16:20 PM	B32: TBA	<b>Kenji Hata</b> National Institute of Advanced Industrial Science and Technology, Japan
16:20-16:45 PM	B33: Electrically Conductive and Thermally Insulative Polymer Nanocomposite Foams for Thermoelectric Applications	<b>Siu Ning Leung</b> York University, Canada
16:45-17:10 PM	B34: Monolithic hierarchical porous carbons and its applications to energy storages and water purification	<b>Peng Wang</b> King Abdullah University of Science and Technology, Saudi Arabia
17:10-17:35 PM	B35: Multi-dimensional carbon fusion bonding for supercapacitor	<b>Seong Chan Jun</b> Yonsei Univeristy, South Korea
17:35-18:00 PM	B36: Carbon Nanotube Nanofluidics: from Fundamental to Applied Science	<b>Francesco Fornasiero</b> Lawrence Livermore National Laboratory, USA
18:00 PM	Dinner Social	
Thursday March 31		
One day academic exchange & excursion		



## EMN Meeting on Carbon Nanostructures

## ABSTRACT SESSION

**A01: Energy storage using carbon-based nanoporous material structures**Jisoon Ihm<sup>1</sup><sup>1</sup>*Department of Physics and Astronomy, Seoul National University, Seoul, Korea**Email: jihm@snu.ac.kr*

Hydrogen is an excellent energy carrier which does not emit carbon dioxide in burning and expected to be one of the alternatives to fossil fuels in the future. However, hydrogen is so bulky in its gas form that an efficient storage of hydrogen is a challenging task in commercialization of hydrogen-fuel-cell-powered vehicles. There exist many nanoporous materials which can potentially be used for hydrogen storage. There have been tremendous efforts to store hydrogen in carbon-based nanomaterials such as carbon nanotubes, but storage under ambient conditions (especially near room temperature) for practical applications has not been successful. We established a consortium with an industry lab and other universities several years ago and have been carrying out research and development[1] to achieve high-capacity molecular hydrogen storage in nanomaterials that can function under practical situations.

Recently, we have focused on studying Alkali-metal inserted graphite oxide(GO) with a large void space for molecular hydrogen storage. It has been found that Alkali-metal ions such as  $K^+$  induce hydrogen polarization and the induced dipole contributes to the binding of  $H_2$  to the system, in addition to the usual van der Waals (dispersion) interaction with GO. It can lead to significant hydrogen storage capacity under ambient conditions. We present a new theoretical model for gas-phase storage in a potential well formed in the pore space, distinct from the conventional model of molecular adsorption at particular binding sites. We are going to report some promising results of hydrogen storage at room temperature in K-intercalated GO using the quartz crystal microbalance method.

1. N. Park, K. Choi, J. Hwang, D. W. Kim, D. O. Kim, and J. Ihm, Proc Natl Acad Sci USA **109**, 19893 (2012).

**A02: Production of Carbon Nanotubes from Graphite via Molten Salt Electrochemistry and their Application in Energy Devices**Carsten Schwandt<sup>1,2</sup><sup>1</sup>*National Chair of Materials Science and Metallurgy, University of Nizwa, Birkat Al Mouz Initial Campus, 616 Nizwa, Sultanate of Oman**Email carsten@unizwa.edu.om*<sup>2</sup>*Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom*  
*Email cs254n@cam.ac.uk*

The production of nano-structured carbon materials is a subject of large scientific and technological interest. A less prominent way of accomplishing this is by the conversion of graphite directly into nanocarbon through the application of molten salt electrochemistry. In this method, alkali metal ions from a molten chloride salt are intercalated into cathodically polarised graphite at a high rate, such that the graphite microstructure is destabilised and various nano-structured carbon species are formed which then detach from the graphite bulk. However, due to the heterogeneous product composition and the low yields, this method has hitherto been regarded as inferior.

This presentation will summarise the research and development work conducted and led by the author that may have the potential to change this view. By rigorously optimising the process parameters and implementing a novel type of process control, it has now become possible to prepare in gramme quantities nano-structured carbon material with nanotube contents as high as 70 to 80%. The nanotubes are multi-walled with varying diameters and occur as entangled aggregates of considerable size. Through a variation of the process, it is also feasible to prepare carbon species filled with tin metal. These have been successfully applied as the anode material in a lithium ion battery.



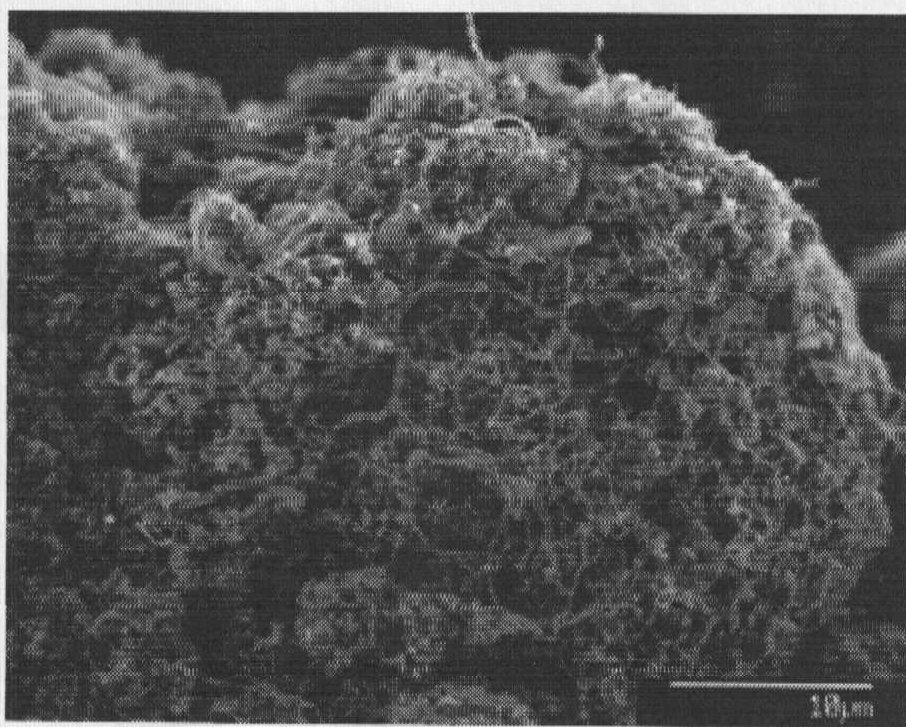


Fig1. Scanning electron micrograph of molten salt electrolytically prepared nanocarbon.

1. C. Schwandt, A.T. Dimitrov, D.J. Fray, The preparation of nano-structured carbon materials by electrolysis of molten lithium chloride at graphite electrodes, *Journal of Electroanalytical Chemistry* **647**, 150–158 (2010).
2. C. Schwandt, A.T. Dimitrov, D.J. Fray, Direct high-yield synthesis of multi-walled carbon nanotubes from graphite by molten salt electrolysis, *Carbon* **50**, 1311–1315 (2012).
3. R. Das Gupta, C. Schwandt, D.J. Fray, Synthesis of tin-filled carbon nano-structures by molten salt electrolysis, *Carbon* **70**, 142–148 (2014).
4. R. Das Gupta, C. Schwandt, D.J. Fray, to be published.

### A03: 3-D nickel-metal layered double hydroxide/CNT nano-architecture composites for high power energy storage application

Zexiang Chen, Yan Wang, Hai Li, Jijun Zhang, Xinyu Yan

School of Opto-electronic Information, University of Electronic Science and Technology of China, 610054 Chengdu, China

Email: zxchen@uestc.edu.cn

Carbon nano tube (CNT) used for supercapacitor electrodes have attracted increasing attention due to their advantages such as high specific surface area, electrical conductivity, strong chemical tolerance, wide working potential window, and excellent utilization rate per quality[1,2]. Meanwhile, pseudocapacitor electrode materials, transition metal hydroxide material have showed excellent

electrochemical properties due to their high reversible redox reactions in the electrode/solution interface, the resulting Faraday pseudo-capacitance is significantly high[3, 4]. In our work, a composite of CNT and nickel-metal layered double hydroxide was firstly prepared in which nano-sheets and nano-rods are attach to the CNT surface forming a 3D structure through a solvothermal method. The SEM and TEM images of the prepared 3D nano structure was shown in Figure 1, and we can see that the nano sheet of nickel-metal layered double hydroxide was grown on the surface of CNT uniformly. Electrochemical measurements were carried out in a three electrode system in 6M KOH solution, with graphite plate and Ag/AgCl as the counter electrode and reference electrode. The specific capacity of the samples is able to reach more than 1000 C/g at the current density of 1 A/g (the corresponding area-normalized capacity is 50.85 C/cm<sup>2</sup>), and the stability is also good comparatively. Especially, the rational design set up a feasible approach to synthesize CNT-based three-dimensional nano core-shell structure.

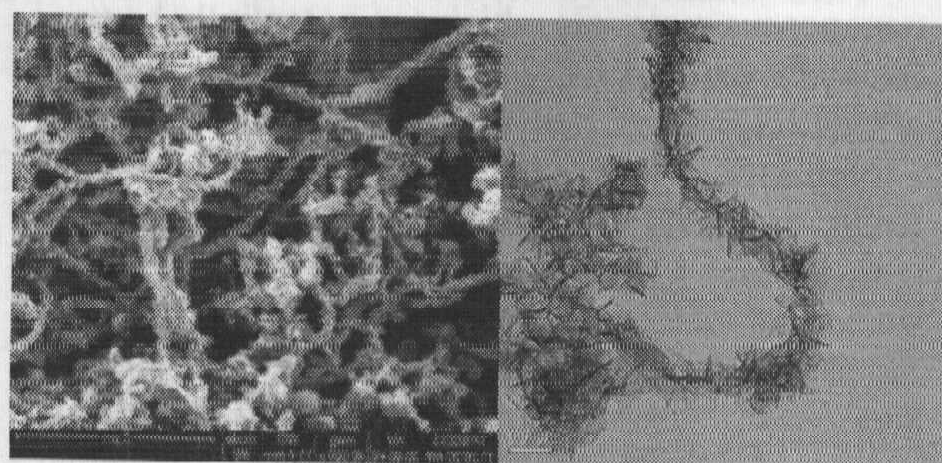


Fig. 1 The SEM and TEM images of as-prepared Ni-Al DHL@CNT composites



1. Z. Tang, C. H. Tang and H. Gong, *Adv. Funct. Mater.* **22**, 1272 (2012).
2. J. W. Zhao, J. Chen, S. M. Xu, M. F. Shao, Q. Zhang, F. Wei, J. Ma, M. Wei, D. G. Evans and X. Duan, *Adv. Funct. Mater.* **24**, 2938 (2014).
3. H. Chen, L. F. Hu, M. Chen, Y. Yan and L. M. Wu, *Adv. Funct. Mater.* **24**, 934 (2014).
4. T. Stimpfling and F. Leroux, *Chem. Mat.* **22**, 974 (2010).

#### A04: Nanocomposite Fabric Sensors for Human Performance Monitoring

Kenneth J. Loh<sup>1,2</sup>, Long Wang<sup>1,2</sup>, Sumit Gupta<sup>1,2</sup>, Helen S. Koo<sup>3</sup>

<sup>1</sup>Department of Structural Engineering, University of California-San Diego, La Jolla, CA, USA  
Email: kenloh@ucsd.edu, web site: <http://armor.ucsd.edu/>

<sup>2</sup>Active, Responsive, Multifunctional, and Ordered-materials Research (ARMOR) Laboratory, La Jolla, CA, USA

<sup>3</sup>Department of Design, University of California-Davis, Davis, CA, USA

Flexible and wearable sensors for human performance sensing have received increased attention, particularly for fitness, healthcare, sports, and military applications. In particular, the measurement of human vital signals provides rich datasets for assessing the subject's physiological or psychological condition, which are directly linked to performance. Instead of using conventional, bulky, wearable transducers, the objective of this study is to design and validate a conformable, non-invasive, and fabric-like sensing system for monitoring body motions, respiration, and temperature. The main sensing element is a piezoresistive multi-walled carbon nanotube (MWNT)-polymer thin film fabricated using spray coating [1]. The films are integrated with stretchable and waterproof fabrics to form the wearable strain sensor.

In total, two types of experimental tests were conducted for characterizing sensor performance. First, the fabric sensors were subjected to uniaxial and cyclic tensile loads and temperature variations. The wearable sensors exhibited stable strain- and temperature-sensitive electrical properties, and high repeatability was demonstrated (Figure 1). Second, upon

characterizing sensor properties (e.g., their sensitivities and calibration curves), the strain-sensitive fabric sensors were adhered onto human subjects for validating human performance monitoring. Here, three sets of tests were performed. The first test utilized a small fabric strip mounted on the individual's index finger to validate sensing of finger movements and bending angles (Figure 2). The second test entailed the design of a chest band that incorporated the nanocomposite fabric sensor. The results showed that sensor electrical properties varied according to chest movements due to respiration activity. The final test investigated these sensors for monitoring distributed pressure. To do so, an electrical impedance tomography (EIT) algorithm was implemented. EIT utilized applied electrical excitations and voltage measurements obtained along fabric sensor boundaries for solving the inverse problem and reconstructing the corresponding 2D spatial distributions of electrical properties [2, 3]. Since the entire fabric was pre-calibrated to strain (and strain induced by out-of-plane applied pressure), EIT outputted the corresponding pressure map. Experiments performed in the laboratory confirmed the applicability of fabric sensors for monitoring pressure distributions (Figure 3). Overall, the proposed wearable fabric sensor design exhibited favorable features such as being flexible, easy to fabricate, light-weight, low-cost, non-invasive, and comfortable to wear.

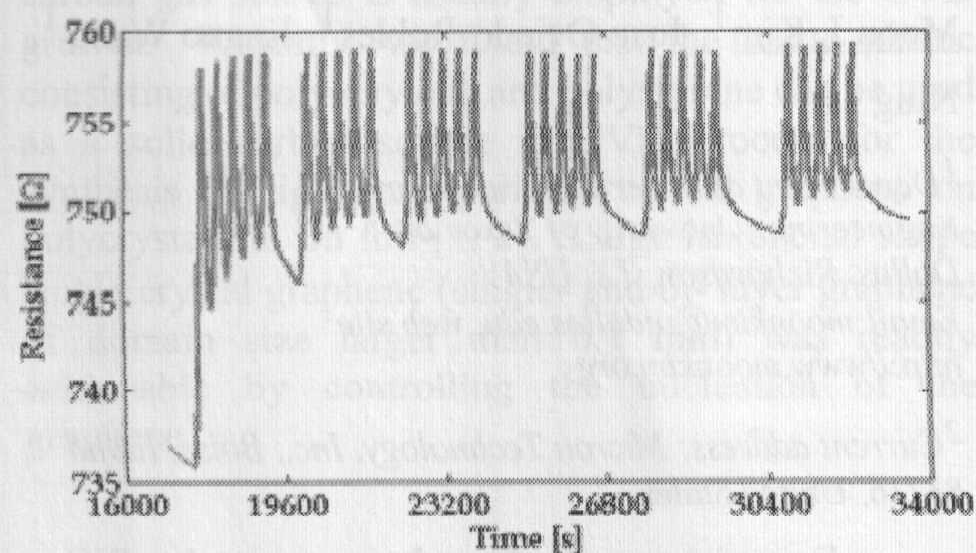
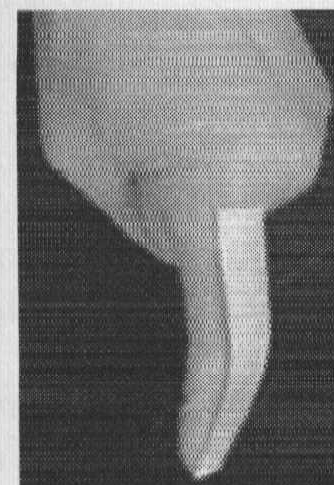


Fig 1 Resistance time history of fabric sensor subjected to tensile cyclic strains.

Fig2. Finger bending monitoring test.





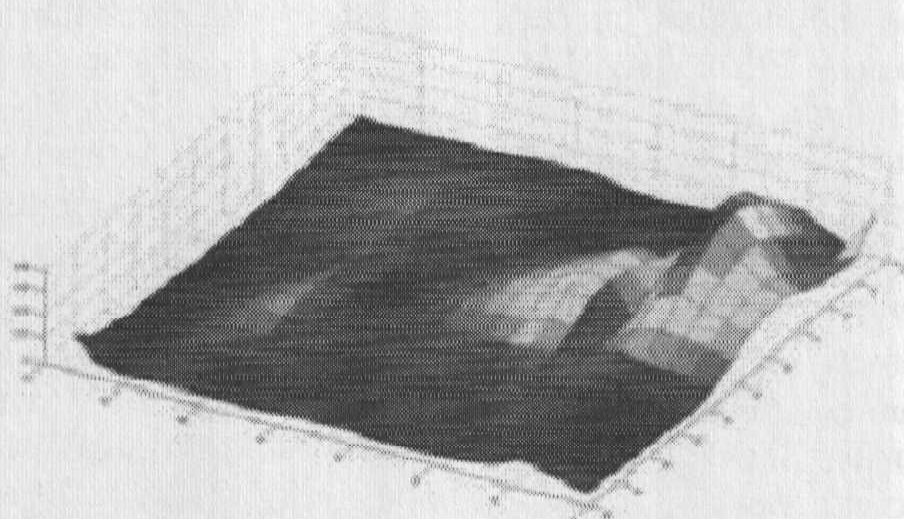


Fig3. Distributed pressure map from fabric sensor measurements and EIT analysis.

1. L. Wang and K.J. Loh, *Science Letters Journal* **5**, 234 (2016).
2. K.J. Loh, T-C. Hou, and J.P. Lynch, *Journal of Nondestructive Evaluation* **28**, 1 (2009)
3. J.G. Gonzalez, S. Gupta, and K.J. Loh, *Proceedings of IEEE* in press (2016).

#### A05: Probing carbon nanostructures for nanoelectronics down to atomic scale

Moon J. Kim<sup>1</sup>, Juan Oviedo-Robles<sup>1</sup>, Jinguo Wang<sup>1</sup>, Ning Lu<sup>2</sup>

<sup>1</sup>Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX, USA  
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Epitaxial growth of graphene on metal or SiC substrates has been demonstrated to be compatible with conventional semiconductor device processing. Challenges in achieving this vision are the control of defect formation and its polycrystalline nature as it is derived from nucleated islands with different orientations that grow together during synthesis [1,2]. This makes synthesis of large single crystal sheets of graphene a major goal for the material. To accomplish this, the mechanisms of growth need to be better understood by analyzing the patterns and behaviors that the graphene lattice exhibits during synthesis.

However, the analysis methods for graphene are very limited due to its sub-nanometer lattice and atomic thickness. The versatility of transmission electron microscopy (TEM) allows for both direct atomic resolution structural imaging and chemical analysis. In particular, scanning transmission electron microscopy (STEM) based analytical techniques has provided not only the elemental identification of impurities and dopant atoms, but also the electronic structure information of defects and edge structures with unprecedented atomic scale resolution. Furthermore, (S)TEM-based *in-situ* techniques such as heating and electrical biasing combined with high energy electron irradiation showed a host of exciting results including the modification of pristine graphene lattice, creation or healing of defects, transformation of graphene to other carbon allotropes, etc.

In this talk, examples of atomic scale characterization of grown graphene (Gr) and its hetero-structure interface with Gr/2D transition metal dichalcogenides (TMDs) will be presented and discussed in the light of nano-electronic applications [3].

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#### A06: Chemically engineered graphene like carbon layers and nanotubes

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We provide theoretical studies concerning the possibility of changing electronic properties of graphene layers and carbon nanotubes (CNTs) through functionalization or forming multiple layers in form of vertical heterostructures or multiple-wall tubes. Our studies are based on the first principles calculations in the framework of the density functional theory. We consider substitution of carbon atoms by nitrogen and boron, decoration of the two studied systems with separate atoms as well as grafting on them simple molecules, such as amines ( $\text{NH}_n$ ) and hydrocarbons ( $\text{CH}_n$ ) at various concentrations. In addition to the case of previously discussed covalently functionalized CNTs, [1-2] we assess the stability of the other functionalized structures and show how the functionalization changes their elastic properties, electronic structure, electric and heat conductivity, and spin properties. Our studies demonstrate that the chemical engineering can lead to materials exhibiting required properties for electronic and optoelectronic devices, such as, for example, graphene based material with finite energy gap, high electric conductivity, and high Young's modulus. Further, employing *ab initio* molecular dynamics, we study the dynamics of chemical reactions leading to chemisorption of some of functionalizing molecules.

We have also studied cohesive transport in functionalized graphene nanoribbons and CNTs employing non-equilibrium Green's function theory in the framework of the density functional theory. Our calculations clearly indicate that functionalization generally diminishes the transmission. However, computed current-voltage characteristics exhibit considerably smaller drop of the current with the concentration of functionalizing molecules in the case of ribbons than tubes. [3]

We address also the important issue for spintronic applications of these materials, namely the possibility to tune spin splitting of bands, and therefore, spin lifetime, through suitable functionalization. We consider also vertical heterostructures consisting of graphene and hexagonal boron nitride layers and demonstrate how various stacking influences the energy gap in these systems.

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#### A07: Dynamic TEM observation of the formation of graphene and carbon nanotubes

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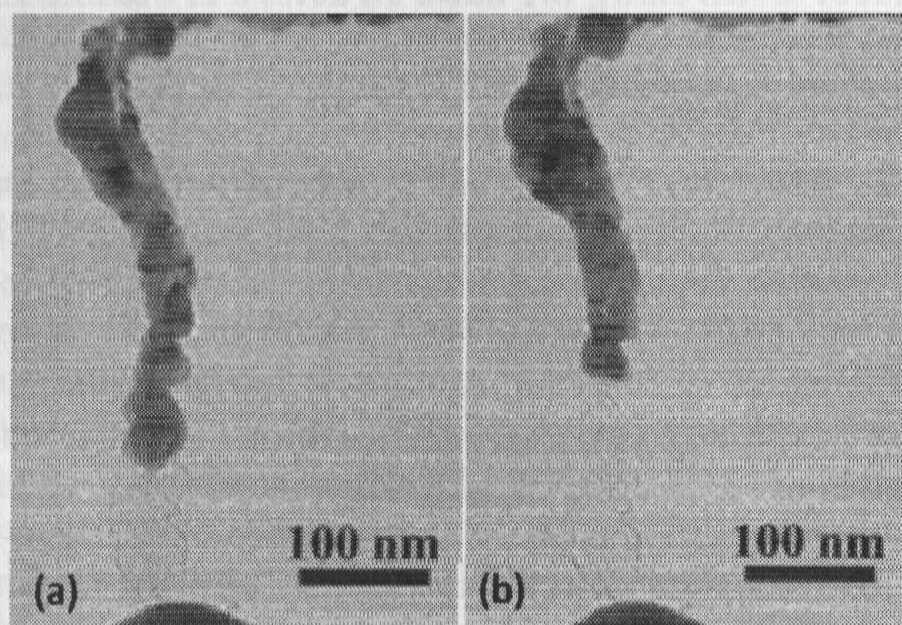
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Low dimensional nano-carbon, such as graphene and carbon nanotubes (CNTs), is one of the hottest materials in nanotechnology and nanomaterials science. A variety of applications is expected due to their exceptional electrical, mechanical, optical, and thermal properties. For graphene, subjects to be solved for realizing those applications include the controllable synthesis of graphene; larger scale synthesis of high quality graphene of larger domain size.

For the large scale synthesis of graphene, chemical vapor deposition (CVD) is promising, and carbon gas source is usually employed for the CVD growth. Recently, we found that the waste plastic consisting of polyethylene and polystyrene can be used as a solid carbon source in CVD process for the synthesis of high quality single crystal graphene on polycrystalline Cu foil [1, 2]. Large hexagonal shape single crystal graphene (single- and bi- layer graphene of domain size larger than 0.1 mm) was readily achievable by controlling the nucleation of the graphene.





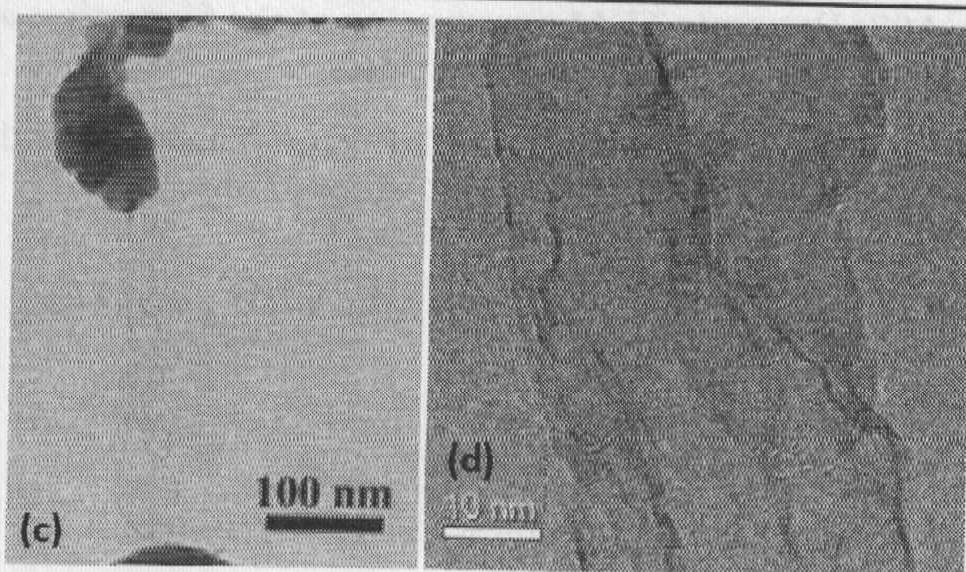


Fig1. (a)–(c) In situ TEM of graphene formation by solid phase reaction. (d) Enlarged TEM image. [3]

To control the graphene growth, its growth process should be well understood. For this purpose, transmission electron microscopy (TEM), which provides the detailed structural information in atomic dimension, is essential. To achieve this, we are tackling also the graphene growth by solid phase reaction. In the talk, visualization (TEM observation in video mode) of graphene formation in nanoscale during the electron current flow will be demonstrated for the Cu-coated and metal included carbon nanofibers, together with in situ CNT formation [3-6].

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#### A08: Controlling the band structure of black phosphorus

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Two-dimensional (2D) atomic crystals have emerged as a class of materials that may impact our future electronics technology [1]. A key issue is controlling their electronic state to overcome the limit of natural properties. In this regard, there are rapidly

growing interests in black phosphorus, a layered material that consists of 2D phosphorene. The low-energy band structure of black phosphorus has been widely predicted to be tunable by various external perturbations, such as applied strain and electric field [2]. In this talk, I will introduce our recent angle-resolved photoemission spectroscopy studies on the tunable band structure of black phosphorus. By the *in-situ* deposition of alkali-metal atoms on the surface of black phosphorus, we found that the vertical electric field from dopants modulates the band gap, and tunes the material from a narrow-gap semiconductor to a band-overlapped semimetal [3]. At the critical density of this semiconductor-semimetal transition, the system becomes a 2D Dirac semimetal, whose band dispersion is highly anisotropic, linear in armchair and quadratic in zigzag directions [3].

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#### B01: Density functional theory calculation for transport property of carbon nanostructures

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Carbon nanostructures, such as graphene, nanotubes, and fullerenes, are known to exhibit a rich variety of electronic structures and are expected to be one of the most promising new materials for future nanoelectronics. For example, carbon nanotubes exhibit various electronic structures from metallic to semiconducting depending on their chirality [1]. The electronic reconstruction of graphenes induced at boundaries can give rise to metal or insulator states, magnetism, or even superconductivity. The discovery of spin-polarized zigzag graphene nanoribbons, in which an opposite spin orientation crosses the ribbon between ferromagnetically ordered edge states on each edge, through theoretical calculations has attracted a great deal of interest in spintronics applications based on graphene based materials [2]. In this talk, I introduce a couple of studies on electron transport property of carbon related materials using first-principles calculations. All calculations are done using RSPACE code [3-5], which bases on the framework of density



functional theory using a real-space finite-difference approach.

### **Transport property of triangular graphene flakes**

The spin polarizations of two dimensional structures composed of boron, nitrogen, and carbon, in which triangular graphene flakes is surrounded by boron nitride sheets (BNC structures), was found by first-principles calculations [6]. Here, spin-polarized electronic structure and transport property of BNC structures sandwiched between graphene electrodes (G/BNC/G structures) are investigated [7]. It is found that the magnetic moment of the graphene flakes increases as the flakes become small and as they are surrounded by a large BN region. The spin polarization of the charge density distribution accumulates at the edges of the flakes and no spin polarizations are observed in the graphene electrodes. Moreover, the first-principles transport calculation reveals that the electron transport through the BNC structure is fully spin-polarized in a wide energy range around the Fermi level. These results indicate that the BNC structure is one of the most promising candidates for electronic control over spin transport.

### **Transport property of a BN ring between carbon nanotubes**

The transport property of the BN ring connected to the carbon nanotube electrode is investigated [8]. The boundary states at the interface between the BN ring and carbon nanotube electrodes lie just below the Fermi level and are energetically dispersionless in a one-dimensional Brillouin zone. However, the contribution of the boundary states to the conductance spectrum is not observed near the Fermi level. By examining the spatial distribution of the boundary states, it is found that the difference in the rotational symmetry between the boundary states and propagating Bloch states from the electrode with respect to the tube axis causes the reflection of the incident electron at the interface. These results indicate that the real-space picture of the scattering wave function is important to interpret transport phenomena in the transition region.

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### **B02: Detection of terahertz radiation by two-dimensional plasmons in lateral carbon nanotube networks**

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We consider the carrier transport and the plasmonic phenomena in the structures with lateral carbon nanotube (CNT) network (CNT "felt"), which can operate as terahertz (THz) detectors. Figure 1 shows the device under consideration. A similar THz detector based on the CNT network was recently fabricated and studied experimentally [1]. We develop the device model for such THz detectors using the lateral CNT networks consisting of a mixture of randomly oriented semiconducting and quasi-metallic CNTs (s- and m-CNTs) with asymmetric contacts (one Ohmic contact and one Schottky contact). The model is based on the concept of the two-dimensional plasmons in relatively dense networks of randomly oriented CNTs and predicts the detector responsivity spectral



characteristics. The detection mechanism is the rectification of the ac current due the nonlinearity of the Schottky contact current-voltage characteristics under the conditions of strong enhancement of the potential drop at this contact associated with the plasmon excitation. The excitation of the two-dimensional plasmons by incoming THz radiation could lead to the sharp resonant peaks of the detector responsivity at the signal frequencies corresponding to the plasmonic resonances.

The obtained theoretical results are compared with the previous [1] and recent [2] experimental data. The proposed device model and its analysis open up the prospects for a substantial improvement of the CNT-based THz detectors.

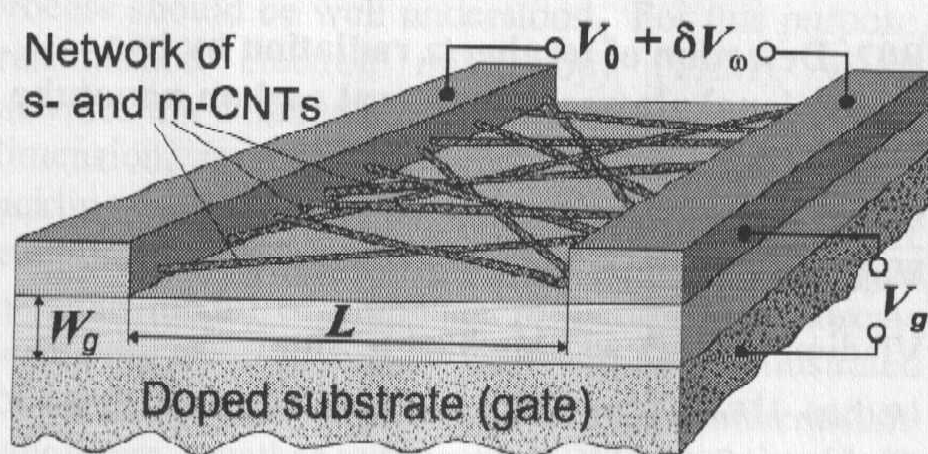


Figure 1 Schematic view of the terahertz detector structure with lateral CNT network.

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### B03: Mechanics modeling on the mechanical and electrical properties of carbon nanotube (CNT)-polymer composites

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Since the discovery of carbon nanotubes (CNTs) [1], the distinguished mechanical and electrical properties of these novel materials have been attracting tremendous attention from research communities. For

example, CNTs have been considered as ideal reinforcement to replace traditional fibers in nanocomposites which could achieve even lighter weight and higher strength [2, 3]. The addition of semiconducting or metallic carbon nanotubes (CNTs) in an insulating polymer matrix for the formation of a semiconducting or conducting composite has been a particular interest for potential stretchable electronics applications [4, 5]. To fulfill the potential applications of CNTs in nanocomposites, it is essential to develop accurate modeling methodology on predicting the overall mechanical and electrical properties of the CNT-based composites.

Regarding the mechanical reinforcement in nanocomposites, understanding the interfacial interactions between the CNTs and the polymer matrix is particularly important since this structure in general possesses a large amount of interfaces due to the small size of CNTs. With the consideration of two interaction mechanisms at the interfaces, i.e., the van der Waals forces and the chemical covalent bonds, an interfacial cohesive law has been developed based on the continuum mechanics modeling. This cohesive law has been incorporated in the micromechanics model to predict the effective mechanical properties of the CNT-polymer composites. Simulation results have revealed that the interfacial behavior has significant effect upon the strength and stiffness of the composites. The CNT size effect has also been illustrated.

In order to more accurately predict the overall electrical conductivity of CNT-polymer composites, a mixed micromechanics model has been developed by incorporating both of their nanoscale and microscale features. Some critical issues related to the conductivity of the nanocomposites have been addressed, including the percolation concentration, stretching effects, conductive networks and electron hopping. Simulation results suggest that both electron hopping and conductive networks contribute to the electrical conductivity of the nanocomposites, while such contribution depends on the CNT volume fraction. Meanwhile, the CNT size effect upon the percolation concentration and the effective electrical property of the composites has also been investigated in the modeling.



In summary, the theoretical models developed in this work are anticipated to provide more accurate prediction on the mechanical and electrical properties of CNT-polymer composites, leading to useful guidelines for the design and optimization of nanocomposites with tuned mechanical and electrical properties.

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#### B04: Simulation Studies of Nanotube Formation by Polymer Adsorption at a Nanowire

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We have used generalized-ensemble Monte Carlo simulation methodologies to investigate the adsorption of polymers at nanowires and nanocylinders [1-3]. For this purpose, a simple generic coarse-grained model for the polymer-substrate system has been employed. One of the major results of the simulations was that tube-like polymer conformations can form spontaneously which resemble boron nanotubes. In this talk, the thermodynamic properties of the structural phases and hyperphase diagrams will be discussed in the spaces of system and external parameters such as adsorption strength and temperature, respectively. Figure 1 shows such a phase diagram for ground states of the system, parameterized by the effective van der Waals wire thickness and the adsorption strength, respectively [1].

Potential applications include nanotube construction and design of tube systems by means of polymers.

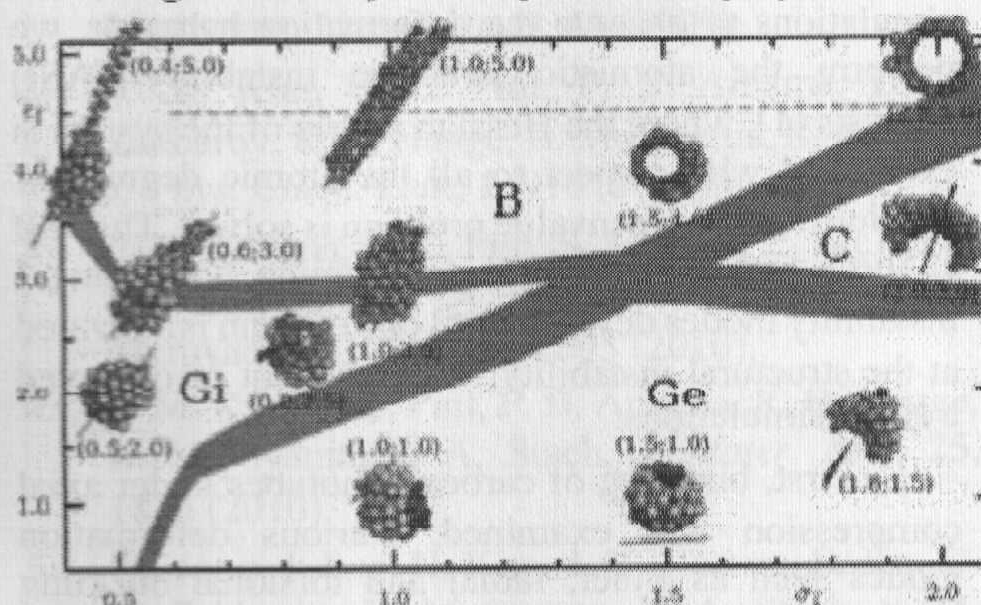


Fig1. Structural phases of a polymer adsorbed at a nanowire.

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#### B05: Atomistic modeling of buckling behavior of pressurized nanotubes

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Buckling is a phenomenon that a structure becomes unstable resulting in a sudden change in its shape when the mechanical load reaches a critical value. As carbon nanotubes exhibit strong coupling between deformation and functional aspects, utilizing the buckling phenomenon may lead to novel nano-devices whose physical properties can be drastically and abruptly changed by a relatively small range of mechanical loading as input. It is therefore of great importance and interest to fully understand the mechanism of buckling of nanotubes under loading.

In this study, we conduct atomistic modeling simulations for carbon nanotubes under radial and axial



compression with the aim to reveal the mechanism of buckling. Besides molecular dynamics (MD) simulations to observe the deformation behavior, we perform the atomistic structure instability (ASI) analysis [1], where the Hessian matrix of the system is calculated with respect to all the atomic degrees of freedom and its eigenvalue problem is solved. The ASI analysis makes it possible to examine how 'latent' instability modes develop until one of them is activated at the structural instability, which cannot be observed by MD simulations.

First, buckling of carbon nanotubes under axial compression was examined. Various deformation modes such as Euler, radial and torsional buckling modes, were found prior to a structural instability. The reduction of Hessian eigenvalues in pristine nanotubes with respect to compressive strain is nearly linear. Change in the radius of nanotubes does not significantly affect the qualitative reduction behavior of each deformation mode but does influence the initial eigenvalues and reduction rates, which clearly explain different buckling behaviors that actually happen at critical strains. A rapid decrease of eigenvalues just before instability was found in models with defects, which is due to localization of instability mode vectors, implying that the nanotube loses mechanical stiffness around defects before instability.

Secondly, buckling of multi-walled carbon nanotubes under radial pressure is investigated. In carbon nanotubes with 4-8 walls, eigenvalues corresponding to buckling of different wave numbers ( $n$ ) show nearly linear reduction with increasing pressure (Fig. 1), which facilitates estimation of the values of critical pressure for the different buckling modes by extrapolation. Similar extrapolation can be made for the number of walls ( $N$ ). For zig-zag nanotubes, buckling with wave numbers larger than 3 (radial corrugation as was predicted by continuum model [2]) is estimated to occur at  $N=15-25$ .

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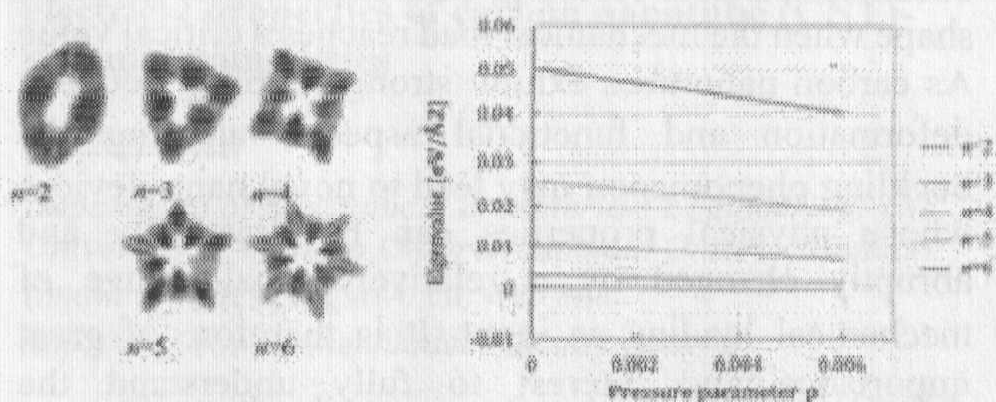


Fig. 1: Eigenvalues of different radial instability modes under increasing pressure in zig-zag MWCNT with  $N=6$ .

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### B06: Tailoring Carbon Nanotube Assembly for Energy Storage Applications

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Sustainable and renewable energy sources from hydropower, solar, and wind power are expected to release the heavy burdens on the current energy infrastructure and the environmental concerns. As these renewable energy sources such as solar and wind power are intermittent in nature, reliable electrochemical energy storage systems, mainly including rechargeable batteries and electrochemical capacitors, are purposely explored to promote efficient utilization of these energy sources and are a growing challenge. The development of high energy storage devices has been one of the most important research areas in recent years and relies mostly on the successful engineering of electrode materials. Carbon nanotubes (CNTs) have been full of surprises since their emergence and are intensively investigated for use as electrode materials in energy storage devices. Utilizing CNTs and their composites for various energy storage applications such as lithium ion batteries and supercapacitors are under scrutiny because of their improved electrochemical activity, cost effectiveness, environmental benign nature, and promising electrochemical performance. In this presentation, I will discuss our research strategies and efforts to employ carbon nanotubes for different energy storage applications including flexible and even stretchable electricity storage devices.

### B07: Investigating Growth Termination Mechanism of Carbon Nanotube Arrays Using Transmission Electron Microscopy Approach



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Since carbon nanotubes (CNTs) have been discovered in 1991, significant research efforts have been devoted not only for synthesizing high quality and structure-controlled CNTs, but also for adapting CNTs into various practical applications in last two decades. Nevertheless, some of the fundamental questions for carbon nanotube growth and growth termination have not been completely answered yet, and this somehow limits widespread usage of carbon nanotubes in real applications. Especially, the limit of CNT lengths makes it very difficult to transfer intrinsic outstanding properties of CNTs into those of macroscopic scaffolds consisting of CNTs. In order to manifest intrinsic properties of CNTs in macroscopic structures, a route to synthesize extremely long CNTs would be one of the most apparent ways. However, CNTs produced by any method so far stop growing after certain lengths are attained. Therefore, with a hope to grow infinitely long CNTs, researchers have investigated growth termination mechanisms of CNT arrays. There have been several growth termination mechanisms proposed to explain various CNT growth termination related phenomena. Our group has proposed a growth termination model in which the evolution in catalyst morphology due to Ostwald ripening and sub-surface diffusion leads to the growth termination of CNT arrays [1-4]. In this presentation, we will briefly introduce the growth termination mechanism based on Ostwald ripening and sub-surface diffusion along with other growth termination mechanisms proposed by other groups. In addition, we recently develop new TEM sample preparation methodology through which we perform in-situ and ex-situ TEM investigation on CNT array growth. Then, we observe new phenomena related to the evolution of catalyst morphology during CNT array growth and propose a modified growth termination model [5]. The modified growth termination model based on new observation will be dealt with in details.

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#### B08: Micro Indentation of densely aligned CNTs film grown on SiC substrate

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The present study describes an indentation response of CNT film grown on SiC substrate by a surface decomposition process. Both single loading and cyclic indentation experiments were carried out.

The CNT film was fabricated on the C-face (0001) of a SiC wafer. Figure 1 shows transmission electron microscope (TEM) and optical images of the CNT film<sup>1</sup>. From the cross sectional image, the lengths corresponding to the film thickness and the diameters of the CNTs were approximately 210 nm and 5 nm, respectively. The structure of the CNTs was a double-walled zigzag structure, as confirmed by x-ray diffraction images. The HREM (high resolution electron microscopy) image in the figure revealed that the CNT growth was directly from the SiC substrate because the CNT was formed by surface diffusion resulting in the evaporation of silicon as silica gas. It is possible to control length and diameter of the CNTs by changing the processing conditions. The CNT density was more than  $10^{10}/\text{mm}^2$ .

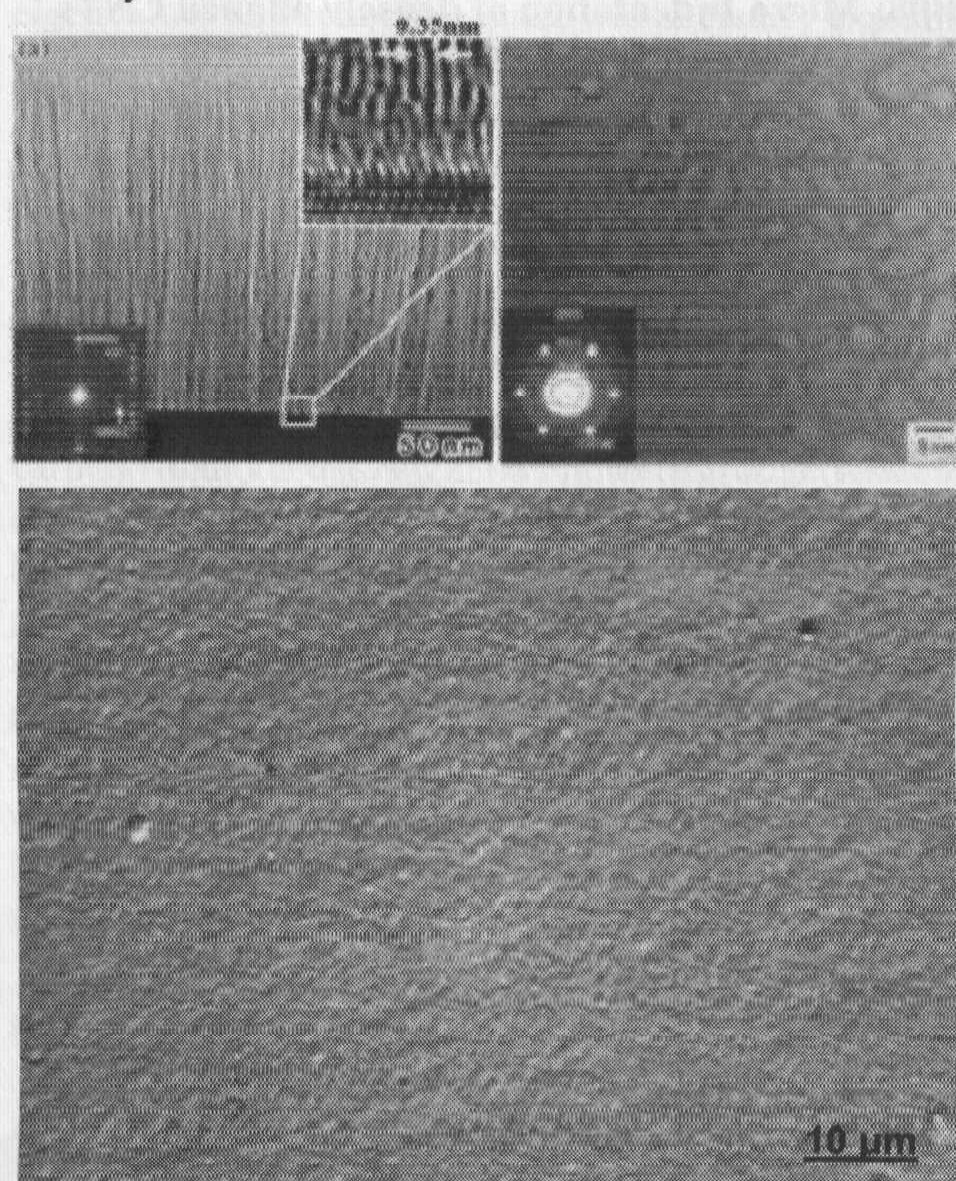


Fig 1. TEM (left and right) and optical (down) images of CNT film

Indentation experiments were carried out with a micro indentation apparatus (DUH 201-WS, Shimadzu Co. Ltd.). Sphere indenters were also used as the tip. As a result, an elastic recovery of the impression was found after a cyclic indentation using a sphere indenter, as shown in Fig. 2.

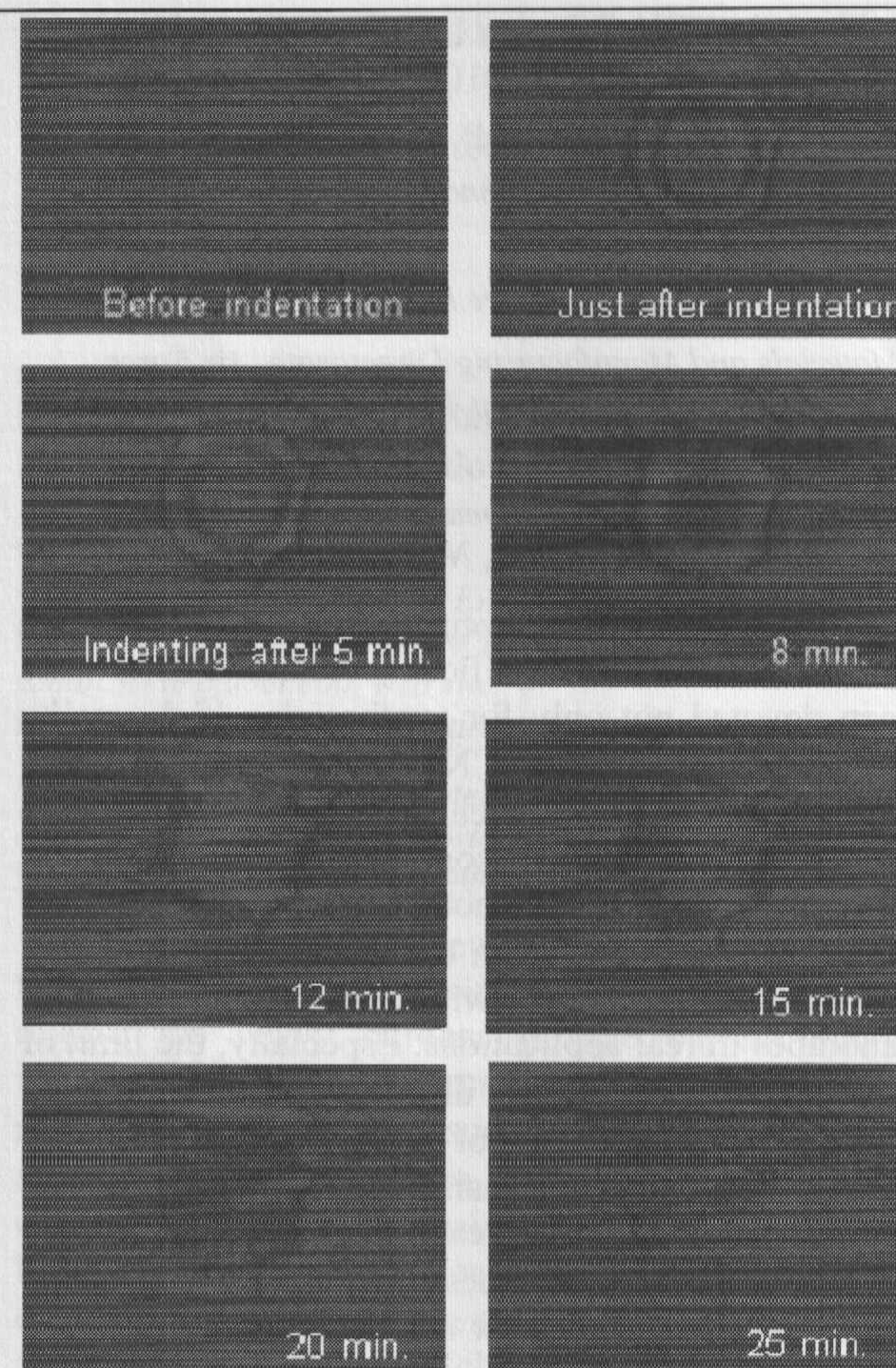


Fig 2. Elastic recovery of impression with sphere indenter

1. M. Kusunoki et al, Appl. Phys. Lett., 77, 531-533 (2000).

#### B09: Biologically assembled conductive nanomesh of single-walled carbon nanotubes for wearable biosensors and devices

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Conductive materials with percolating structures have been attracting tremendous interest in the fields of stretchable electrodes, transparent conducting electrodes, energy storage/conversion devices,



wearable electronics and sensors, and bio-interfacing materials. Percolating structures can provide large effective surface area of electronic materials, enabling efficient interfacing with ionic systems such as biological, biochemical, and electrochemical systems as well as mechanical flexibility. Single-walled carbon nanotubes (SWNTs), rolled-up sheets of graphene, are attractive nanoscale electronic materials for fabricating percolating conductive materials owing to their extremely large aspect ratio and excellent electrical and mechanical properties.

In this talk, a biological material-based method to assemble conductive nanomesh of SWNTs in solution and produce patterns of SWNT-nanomesh on flexible substrates with excellent control of nanostructures will be presented. In our approach, a genetically engineered filamentous M13 phage with strong binding affinity toward SWNTs controls and stabilizes the nanostructures of the SWNT-nanomesh during a hydrodynamic process.<sup>1,2</sup> This unique biological material-based in-solution assembly process enables the realization of conductive nanomesh of SWNTs, independent of the substrate, as well as the delivery of intact nanostructures onto large-scale flexible devices. We demonstrate that the assembled SWNT-nanomesh, integrated into a 40-channel flexible microarray and used for high-density electroencephalography (EEG) on a mouse skull, greatly reduces the in vivo contact impedance and significantly increases the detection rate of high frequency brain signals (HFBS) that are low in amplitude and have been studied mainly by using invasive electrodes.<sup>1</sup> We also show that nanomesh-based nanostructured enzyme platform can be successfully realized in combination of specific biomolecular attraction and electrostatic coupling of the nanomesh.<sup>3</sup> Direct-electron-transfer (DET) of enzymes with various types of catalytic activities is realized and DET-based flexible biosensors are also presented. Active electronic devices based on the nanomesh will be also presented.

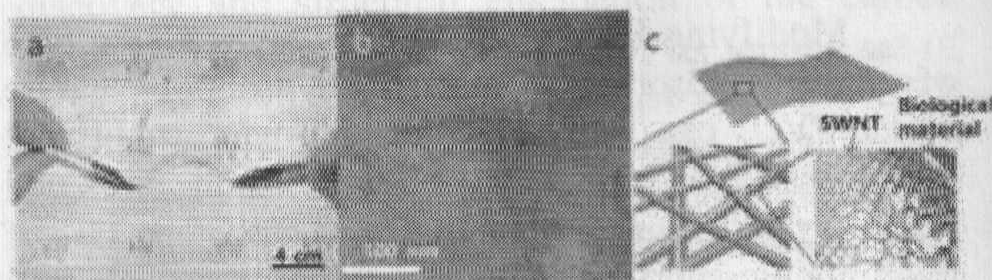


Figure. 1 a) Photograph of the conductive nanomesh freestanding in water, b) High-resolution TEM of the nanomesh, c) Schematic of the binding scheme of the nanomesh.

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2. S. M. Ju, *et al.*, *Scientific Reports*, **5**, 9196 (2015)
3. S.-W. Lee, *et al.*, *Adv. Mater.* DOI:10.1002/adma.201503930.

### B10: Thermo/Piezo – Electric Power Scavenging Using Carbon Nanotube Composites

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The use of organics for waste power recovery usually focuses on a single set of properties useful for the purpose: thermoelectric, piezoelectric, pyroelectric, etc. And while organics may offer textile-like formats that promise the ubiquity of a cloth, they still have a ways to go in power density. Our work focuses on thermo/piezo-electric generators or TPEGs, which integrate two orthogonal power scavenging modalities; thermoelectrics and piezoelectrics. Through the use of carbon nanotube matrix composites, and simple topological constructs, a novel energy harvesting system emerges that can collect power from both kinetic and thermal sources. Such structures have shown synergistic effects between the modalities that yield a greater overall power output than would be expected from either individually. That is, when the structure undergoes simultaneous thermal and kinetic activation, the total power output is larger than the simple addition of the thermoelectric components and the piezoelectric components separately. We have now shown that these TPEG synergistic effects are derived from an internal “field-doping” of the reduced-dimension CNTs. Specifically, singularities within the electronic band structure of the CNTs, can be used to dramatically increase the thermoelectric output when internal voltages are presented by the piezoelectric. This talk will explore a range properties seen in these new hybrid thermo/piezo electric systems as well as their implications in a host of applications.



Figure 1 shows a schematic of one of the hybrid structures to achieve the synergistic TPEG effect. The piezo between the two doped, nanotube thermoelectric sheets acts to apply an internal field across the nanotubes thereby modifying their thermoelectric properties. This talk will discuss the thermodynamic implication of this system.

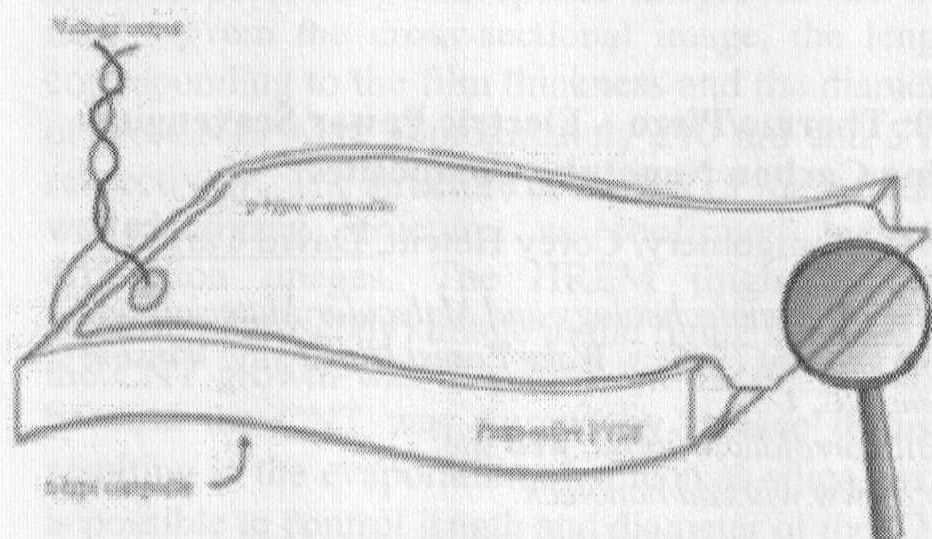


Fig1. The TPEG

### B11: Megagauss Magneto-optical Survey of Exciton States in Single-wall Carbon Nanotubes

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Single carbon nanotubes with a typical tube diameter an order of 1 nm and the length an order of 100 nm, are characterized by the quasi-one dimensional system. Optical properties are enriched by the enhanced excitonic band-edge structure. When a magnetic flux penetrates through the tube, the electronic band structure is subjected to substantial modulation via the mechanism of Aharonov-Bohm (A-B) effect, which is called A-B splitting. This effect lifts the quantum degeneracy of the band-edge states, induces splittings of the exciton optical absorption peak in megagauss magnetic fields, which depends much on fine structure of the excited energy states. What is very important in an opto-electronic engineering application is, for example, the relative ordering of the optically accessible and non-accessible states, i.e. bright and dark exciton states, which are critical for the optical radiative and non-radiative recombination processes of photo-excited carriers. The magneto-optical A-B splitting was investigated in magnetic fields of up to 300 – 400 T, and it was found that the relative ordering of bright and dark states is

determined by the specific chirality of carbon nanotubes. Our study also demonstrated that the A-B splitting contains the microscopic information of environment substances around the carbon nanotubes.

### B12: Carbon Capture using Waste Polymers Supported on SBA-15 silica and other Nanoporous Materials

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Emission of carbon dioxide has been widely linked to climate change and this problem must be addressed. “Carbon Capture”, a process to remove CO<sub>2</sub> from flue gas, has offered one solution to reduce CO<sub>2</sub> emission from large-scale industries, e.g. power stations and oil/gas industries. Currently technology in carbon capture using liquid amine is energy intensive in absorbent regeneration as most energy was spent on heating up water (90% in absorbent). Consequently, research on solid state CO<sub>2</sub> adsorbents (e.g. MOFs, zeolites) has flourished in recent years.[1]

In this presentation, we introduce the use of waste polymers for carbon capture. Waste polymers (chitosan and PVC) themselves possess environmental issues upon disposal. Making use of them would be welcome by environmentalists. Since these polymer adsorbents have low surface area, supporting them on a high surface area support is essential for enhancing the CO<sub>2</sub> adsorption capacity. In our work, we have shown that supporting chitosan on SBA-15 silica can increase the adsorption capacity by 20 fold. [2]

Modifying PVC using amines gives a new type of polymeric adsorbents. Due to its hydrophobic nature, amine-PVC can have advantage over traditional hydrophilic adsorbents, e.g. zeolites and aminated silica, if the flue gas has a higher water content. Use of hydrophobic supports including carbon materials will also be studied.



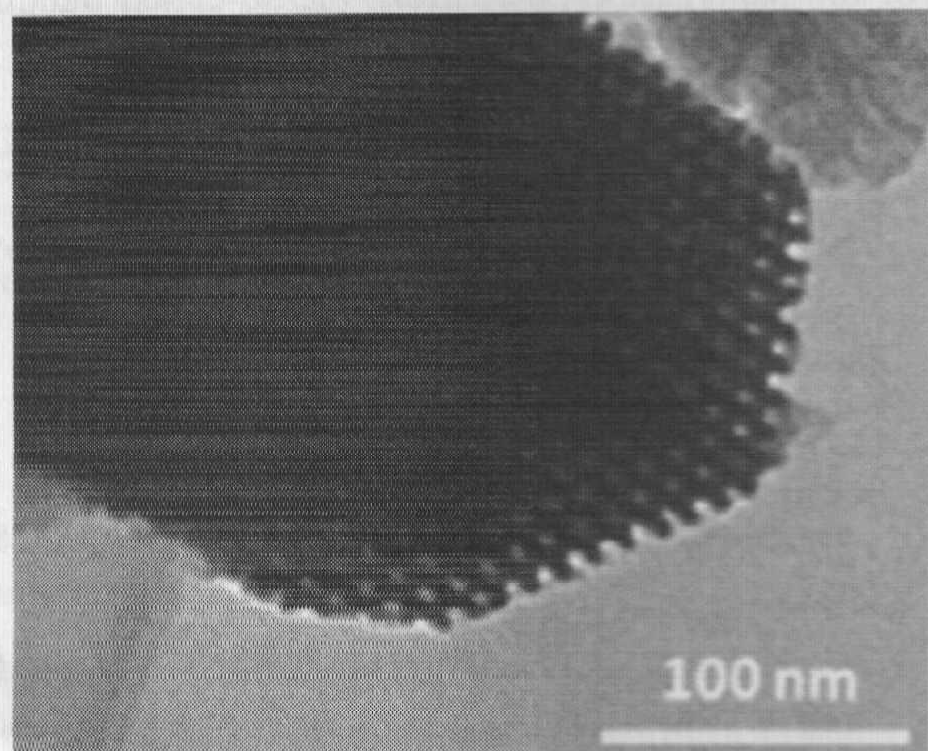


Fig1. TEM image of SBA-15 with a hexagonal array of "nanotube" structure.

1. G. Sneddon, A. Greenway, H. H. P. Yiu, *Adv Energy Mater* 1301873 (2014).
2. G. Sneddon, A. Y. Ganin, H. H. P. Yiu, *Energy Technol* 3, 249 (2015).

### B13: Towards Realizing a SWCNT Industry from Fundamental Science

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Over two decades have passed since the report discovery and structural elucidation of the carbon nanotube (CNT), the application of its unique set of properties have yet to reach industry. While CNT commercial applications grows closer to a reality with new innovations every year, there remains much still to be learned about the synthesis process. This presentation will provide a description of our research on single-wall carbon nanotube (SWCNT) synthesis development, scaling-up, and the establishment industrial-level mass production plant. This work centers on our core technology of water-assisted chemical vapor deposition technique, a method which realizes the highly efficient synthesis of vertically

aligned SWCNTs grow from substrates (SWCNT forests). In one section, I will briefly present the initial development of this synthesis method and its scale-up. In addition, I will describe our efforts for the synthetic control of SWCNTs and the intrinsic requirements for the formation of a single-wall carbon nanotube forest while maintaining high growth efficiency, and its impact on the unique set of CNT characteristics, which is necessary for the development of applications and mass production technology.

This paper is based on results obtained from a project commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

### B14: Development of fluorescent graphene quantum dots for bioimaging

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A facile bottom-up method for the synthesis of highly fluorescent graphene quantum dots (GQDs) has been developed using a one-step pyrolysis of a natural amino acid, L-glutamic acid, with the assistance of a simple heating mantle device. The developed GQDs showed strong blue, green and red luminescence under the irradiation of ultra-violet, blue and green light, respectively. Moreover, the GQDs emitted near-infrared (NIR) fluorescence in the range of 800-850 nm with the excitation-dependent manner. This NIR fluorescence has a large Stokes shift of 455 nm, providing significant advantage for sensitive determination and imaging of biological targets. The fluorescence properties of the GQDs, such as quantum yields, fluorescence life time, and photostability, were measured and the fluorescence quantum yield was as high as 54.5 %. The morphology and composites of the GQDs were characterized using TEM, SEM, EDS, and FT-IR. The feasibility of using the GQDs as a fluorescent biomarker was investigated through *in vitro* and *in vivo* fluorescence imaging. The results showed that the GQDs could be a promising candidate for bioimaging. Most importantly, compared to the



traditional quantum dots (QDs), the GQDs is chemically inert. Thus, the potential toxicity of the intrinsic heavy metal in the traditional QDs would not be a concern for GQDs. In addition, the GQDs possessed an intrinsic peroxidase-like catalytic activity that was similar to the graphene sheets and carbon nanotubes. Coupled with 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid) (ABTS), the GQDs can be used for the sensitive detection of hydrogen peroxide with a limit of detection of 20  $\mu\text{M}$ .

### B15: Anomalous enhancement of Seebeck coefficients for the graphene/h-BN composites

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The thermoelectric conversion has been of interest for many researchers since Hicks and Dresselhaus showed that the introduction of low-dimensional structures such as quantum well structures would significantly enhance the dimensionless figure of merit [1]. Graphene is a two-dimensional, monolayer material having honeycomb lattice of carbon atoms and has significant thermal properties [2,3]. It has been suggested that the graphene-based device can be a novel thermoelectric material because of its potential giant Seebeck coefficient larger than 30 mV/K [4]. On the other hand, graphene nanoribbon (GNR) is a one-dimensional (1D) material, a strip of graphene, which has also been investigated theoretically as thermoelectric materials. A molecular dynamics study has shown that a high figure of merit can be obtained for the zigzag GNR (ZGNR) [5]. This result implies that the introduction of 1D structural modulation makes graphene into novel thermoelectric materials. We hereby propose, in this study, superlattice or composite models consisting of ZGNR and zigzag BN nanoribbon (ZBNR) [6].

Figure 1 shows the structure of a ZGNR/BNNR superlattice. We have investigated the Seebeck coefficients of ZGNR/BNNRs within the Boltzmann transport theory. It has been confirmed that the Seebeck coefficients of ZGNR/BNNRs are drastically enhanced from those of ZGNRs as shown in Fig. 2 [7]. It has been revealed that the giant Seebeck coefficients

of the superlattices stem from the so-called pudding mold band with a finite energy gap.

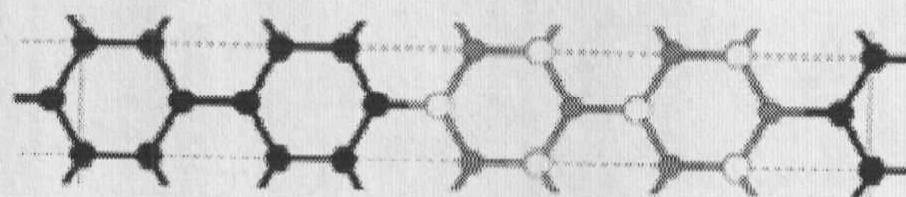


Fig. 1 Structure of (4,4)ZGNR/BNNR; Black, white, and gray balls indicate C, N, and B atoms, respectively. The polar interfaces are formed between ZGNR and BNNR.

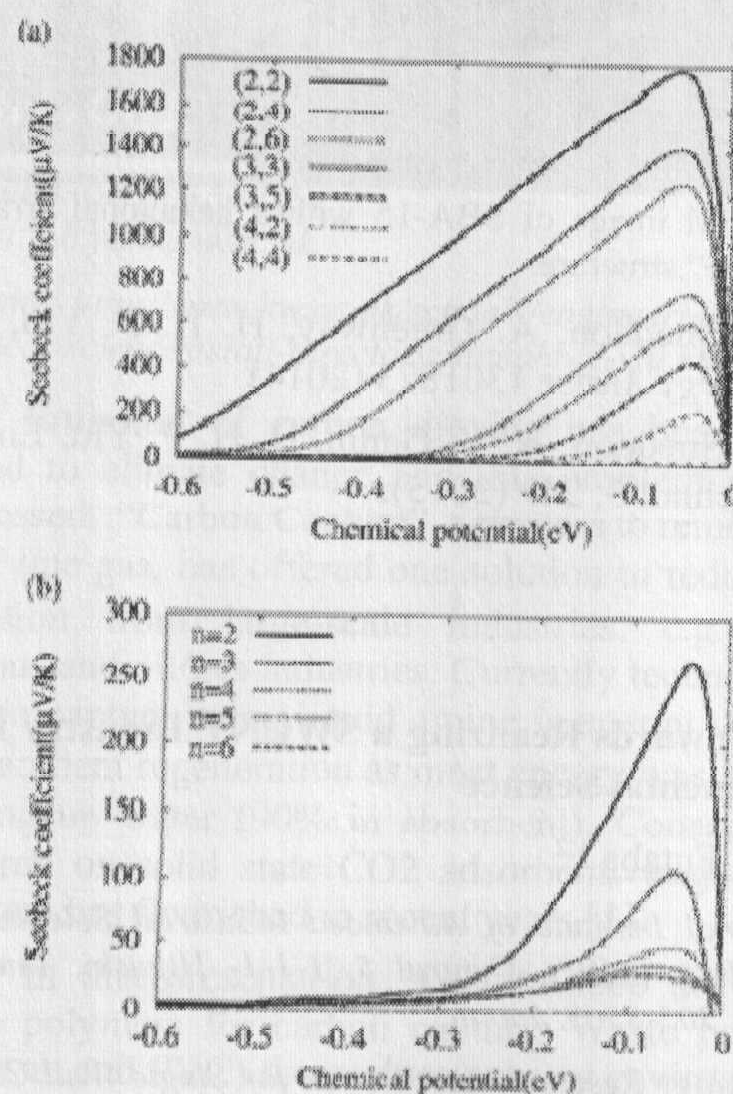


Fig. 2 Seebeck coefficients as a function of the chemical potential for (a) the 2D ZGNR/BNNR superlattices and (b) 1D ZGNRs.

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3. E. Watanabe, S. Yamaguchi, J. Nakamura and A. Natori, Phys. Rev. B **80**, 085404 (2009).
4. D. Dragoman and M. Dragoman, Appl. Phys. Lett. **91**, 203116 (2007).



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### B16: Quantum interference effects in graphene nanostructures

Adam Rycerz and Grzegorz Rut

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Selected graphene nanostructures, including rings and disks, preserve the peculiar feature of bulk graphene, in which any quantum state appears in two copies (on per each valley in the dispersion relation), link by the time-reversal symmetry (TRS). For this reason, such structures were considered theoretically as possible building blocks for a solid-state quantum computer, as weak magnetic field breaking the TRS can be used to lift out the valley degeneracy, and to control a valley qubit [1]. Both experiment and computer simulation of quantum transport through the ring, displaying Aharonov-Bohm-like oscillations, suggested the robustness of a valley pseudospin [2,3].

In stronger magnetic field, Aharonov-Bohm effect in graphene ring disappears, as the two arms are no longer equivalent due to the Lorentz force. Surprisingly, theoretical analysis of the Corbino geometry, in which a disk-shaped sample area is attached to the circular leads, suggests that periodic magnetoconductance oscillations should be observable provided the electrochemical potential is adjusted to any Landau level [4,5]. We further predicted that such effect has a direct analog in bilayer graphene, in which peculiar features of magnetotransport can be used to determine the value of skew-interlayer hopping [6], a tight-binding model parameter difficult to estimate with available experimental techniques.

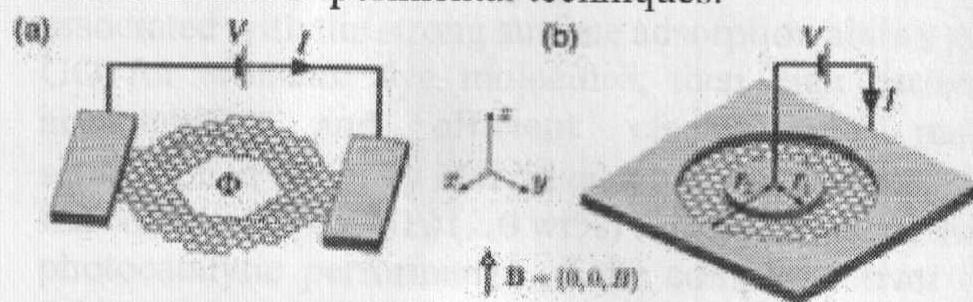


Fig 1. Devices considered in the presentation (schematic). Voltage source passes the current from the right to the left lead in case of the Aharonov-Bohm ring (a) or from the outer circular lead to the inner one in case of the Corbino disk (b) in graphene. Additional gate electrodes (not shown) may be used to tune dopings or to induce transverse electric fields. [Reprinted from: A. Rycerz, Acta Phys. Polon. A **121**, 1242-1245 (2012).]

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### B17: In-situ Raman spectroscopy of graphene thin films containing palladium particles at the presence of hydrogen atoms

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In-situ Raman spectroscopy of flexible graphene-oxide films examined upon exposure to hydrogen gas, air and synthetic air. The changes in D and G peaks are attributed to defects responding to atomic hydrogen spilled over from the catalytic behavior of Pt nanoparticles distributed all over the film. High resolution transmission electron microscopy images (HRTEM) as well as electron energy loss spectroscopy (EELS) were carried out to define the density of the samples.

Graphene samples were previously synthesized at UCLA [1] using Laser Scribed Graphene (LSG) from high purity graphite powder on polyethylene terephthalate (PET) as a flexible substrate. HRTEM (Fig. 1) and EELS are carried out using JEOL 2100F electron microscope. The K-edge spectrum quantified in order to find out the oxygen fraction in the films and the density of the films [2].

The Raman spectra of the sample in three



different environments a) air, b) synthetic air and c) 1%  $H_2$  in synthetic air collected at room temperature are presented in Fig. 2. As can be seen strong D and G peaks occur at about  $1360\text{ cm}^{-1}$  and  $1560\text{ cm}^{-1}$  respectively for visible excitation. The shift in the G peak could be explained as the changes in bonding structures mainly formation of H-C bonds on dangling bonds or on the edges.

We have performed in-situ Raman spectroscopy to graphene-oxide layers containing Pt nanoparticles to investigate the effect of atomic hydrogen at room temperature. There is a significant change in the G and D peak magnitudes as the sample expose to  $H_2$  and air attributed to the formation or removal of C-H bond on the edge or dangling bond responding to atomic hydrogen spilled over from Pt nanoparticles [3].

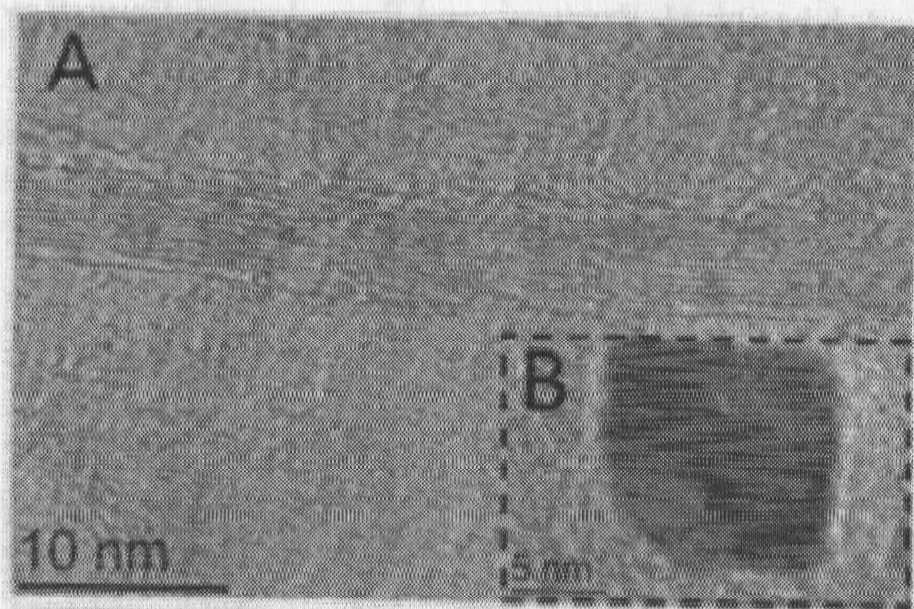


Fig. 1: A) Plan view image of the layer. B) HRTEM image of a Pt nanoparticle on graphene-oxide

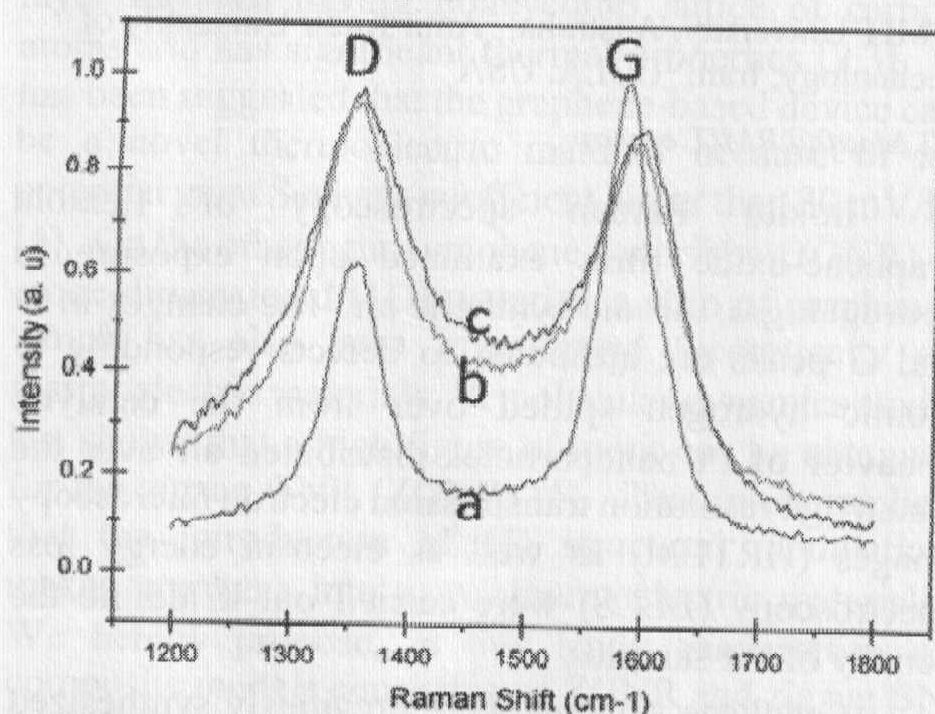


Fig. 2: The Raman spectra of the sample in three different environments; a) air, b) synthetic air and c) 1%  $H_2$  in synthetic air collected at room temperature

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### B18: Ag Nanoparticles/ Graphene Oxide (GO)/ $\alpha$ - $Bi_2O_3$ Hybrid Versatile Composites for Visible Light Photocatalysis and Chemical Catalysis

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The growing challenges of environmental purification by solar photocatalysis and precious metal free catalysis are receiving the utmost global attention. In these regards, composite materials based on graphene and graphene-oxide are being considered to be significantly promising. GO structurally constitutes of the graphene framework with some oxygen containing functional groups like the hydroxyl, epoxide, phenolic-OH and carboxylic groups that are attached at the basal planes and edges of the hexagonal carbon framework. These ionisable functional groups present on GO, act as binding sites facilitating the deposition and anchoring of nano-semiconductors, metal nanoparticles (NPs) and organic (dye) molecules via direct non-covalent, covalent,  $\pi$ - $\pi$  and/or van der Waals interaction.

Here we demonstrate the large economical scale fabrication of a new eco-friendly composite material- $\alpha$ - $Bi_2O_3$  micro-needles intercalated with anchored graphene oxide (GO) micro-sheets (1.0 wt%) –for the above mentioned applications formed via a single-pot green chemical hydrolysis reaction. The incorporation of plasmonic Ag (2 wt%) nanoparticles (NPs) is further seen to improve the performance of the composite.



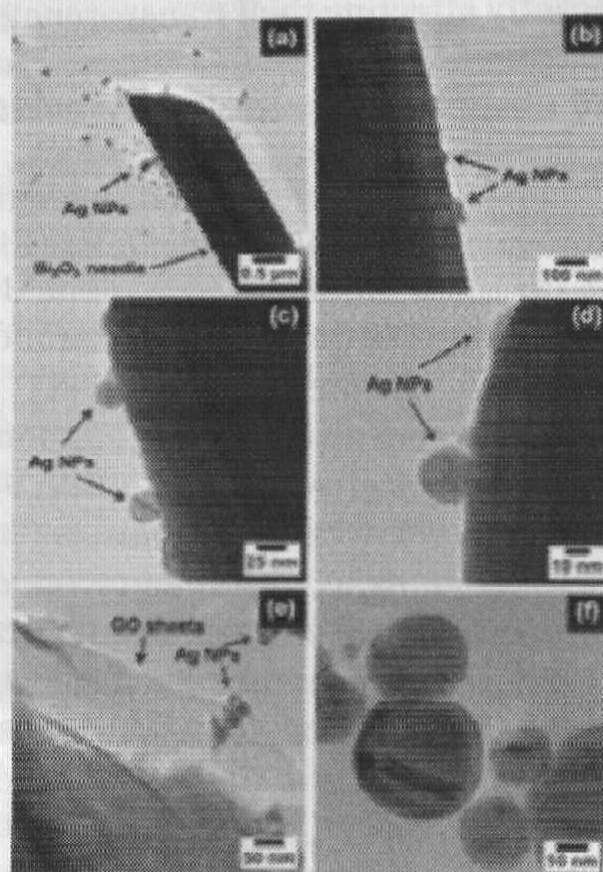


Figure 1. TEM images of the sample Ag/GO/Bi<sub>2</sub>O<sub>3</sub> showing (a)  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> needles and Ag NPs, (b-d) Ag NPs strongly attached on to the surface of the  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> needle, (e) Ag NPs located on the surface of the GO sheets and (f) near-spherical Ag NPs at a higher magnification (image adapted from Ref. 1)

The size and morphology of the synthesized photocatalysts is determined by scanning and transmission electron microscopy. The  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> is seen to have a needle-like morphology. The length of the needles ranges from 5 to 25  $\mu$ m and the diameter is typically about 1  $\mu$ m. The SEM images of the GO hybridized composites show randomly oriented Bi<sub>2</sub>O<sub>3</sub> needles intercalated with transparent GO sheets. The TEM images (Fig 1) show the presence of near-spherical Ag NPs strongly attached to the  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> needle surface and anchored on crumbled GO sheets. The size of the Ag NPs are found to vary widely from about 2 – 70 nm.

The bare  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> micro-needles display twice as better photocatalytic activities than commercial TiO<sub>2</sub> (Degussa-P25) while the GO hybridized composite exhibit ~4-6 times enhanced photocatalytic activities than neat TiO<sub>2</sub> photocatalyst in the degradation of colored aromatic organic dyes (crystal violet and rhodamine 6G) under visible light irradiation (300 W tungsten lamp). The highly efficient activity is associated with the strong surface adsorption ability of GO for aromatic dye molecules, then high carrier acceptability and efficient electron-hole pair separation in Bi<sub>2</sub>O<sub>3</sub> by individual adjoining GO sheets. Introduction of Ag NPs (2.0 wt%) further enhances the photocatalytic performance of the composite over 8 folds due to a plasmon-induced electron-transfer

process from Ag NPs via GO sheets into the conduction band of Bi<sub>2</sub>O<sub>3</sub>. The new composites are also catalytically active. They catalyze the reduction of 4-nitrophenol to 4-aminophenol in presence of borohydride ions. Photoanodes assembled from GO/ $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> and Ag/GO/ $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> composites display an improved photocurrent response (power conversion efficiency ~ 20% higher) over those prepared without GO in dye-sensitized solar cells.

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### B19: Self-assembled nanotube with enzymatic functionality

Junqiu Liu Jiayun Xu

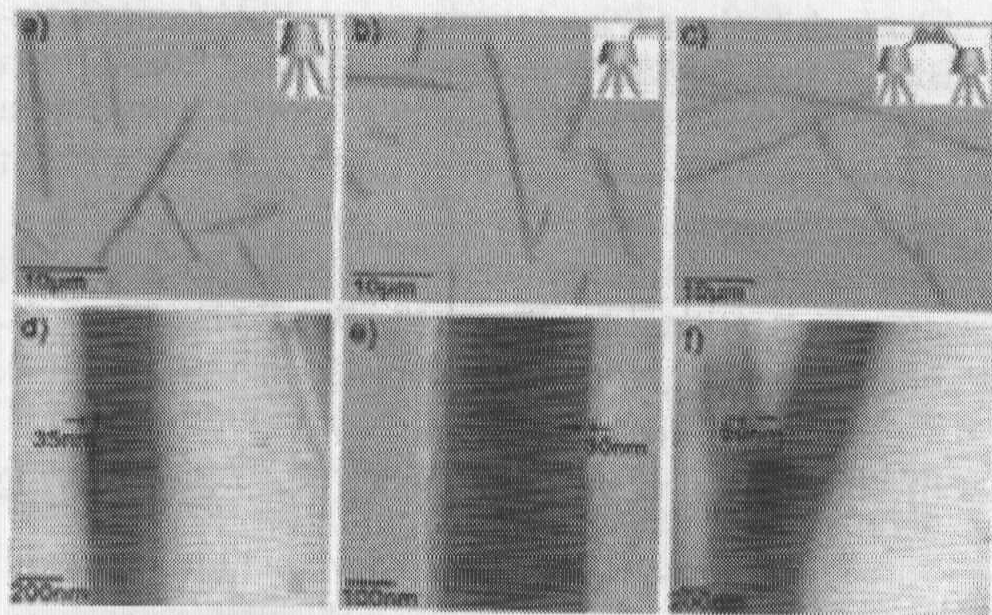
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In recent years, supramolecular amphiphiles formed through noncovalent driving forces have been developed as a new type of building block for future fabrication of supramolecular architectures through multilevel self-assembly. Among them, host-guest interactions, such as those of cyclodextrin (CD) systems, have proven to be important for constructing supramolecular amphiphiles. The self-assembly of host-guest superamphiphiles can provide opportunities not only for structural versatility but also for functional modulation of nanomaterials such as nanotubes. The easy introduction of enzyme catalytic moieties on host or guest molecules would provide an important tool to functionalize the self-assembled nanostructures.

In this talk, we report a novel way to construct giant nanotubes triggered by direct self-assembly of CD-based host-guest superamphiphiles. The spontaneously formed nanotubes were functionalized with the catalytic moieties of glutathione peroxidase (GPx) by modifying the host molecule CD. Furthermore, by manipulating the surface of the nanotubes, nanotube structures can be changed from straight to branched, and can also change from nanotubes to vesicles. We demonstrated that CD-



based self-assembly of supramolecular amphiphiles has great potential for the construction of functional nanomaterials and could become a powerful tool to modulate enzymatic functions on nanotubes.



### Acknowledgements

This work was supported by the Natural Science Foundation of China (no. 21234004, 21420102007, 21574056, 21221063), and the Chang Jiang Scholars Program of China.

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### B20: Self-assembled Films of Polyaniline and Carbon Nanotubes: their use as transparent electrodes and gas sensors

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The synthesis and characterization of thin films of polyaniline/carbon nanotubes nanocomposites is presented, as well as their use as transparent electrodes in ITO-free organic photovoltaic devices and gas sensors. These films are generated by interfacial synthesis, which provides them with the unique ability to be deposited onto any substrate. Very high carbon nanotube loadings can be achieved using these films

without significantly affecting their transparency ( $\approx 80-90\%$  transmittance at 550 nm). Sheet resistances as low as  $300 \Omega/\square$  are obtained using secondary polyaniline doping in the presence of carbon nanotubes. These films present excellent mechanical stability, exhibiting no lack in performance after 100 bend cycles. Flexible and completely ITO-free organic photovoltaic devices are built using these films as transparent electrodes, and efficiencies (up to 2%) are achieved. [1] These nanocomposites films were also tested as ammonia gas sensors and the device's sensitivity was studied concerning three different doping approaches (sulfuric acid, camphorsulfonic acid and m-cresol). The polyaniline high sensitivity to ammonia combined with the stability of the carbon nanotube net increased the reproducibility when compared to sensors based on regular polyaniline. The sensor in which the doping was performed by the use of camphor sulfonic acid, presented the relative better sensitivity for ammonia gas (418%) when compared to the others. This result is addressed to the better polymer configuration achieved by this procedure.

In order to understand how the charges are transported in thin films of polyaniline and nanocomposites with carbon nanotubes we perform a study on the morphological and electrical properties of these films. The polyaniline in this case is chose to be without doping. From electric conduction analyses that explain the  $I-V$  experimental curves, we proposed an adapted model of fibrillar conduction path to calculate the electrical transport in PANI-CNT composites for different carbon nanotube mass fraction, in which the composites are treated as two conductivity domains whose transport is limited by tunneling through PANI barriers. This study demonstrates that by increase of the amount of carbon nanotubes in the nanocomposite films, the electrical conductivity can increase up to 5 orders of magnitude if compared to the pure polyaniline film, presenting a percolation limit of around 1% of carbon nanotubes by mass, and the calculations allow us to predict the length of PANI barrier for tunneling between 11 and 15 Å of PANI as a function of the carbon nanotubes concentration in the films. [3]

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### B21:Forming CNT-Guided Stereocomplex Networks in Polylactide-Based Nanocomposites

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Grafting a nanoparticle surface using a polymer similar to the matrix has been widely applied to control the spatial organization of nanoparticles. However, the fabrication of target materials with well-defined nanoparticle arrangement remains fundamentally difficult because of the absence of specific interactions between the matrix and the graft. [1,2]

In this study, the self-networking structure of poly(D-lactide)-grafted carbon nanotubes (CNT-g-PDLA) in poly(L-lactide) (PLLA) matrix was investigated. Specific interactions between enantiomeric pairs not only promoted CNT dispersion, but also contributed to the regular phase-separation-like CNT self-networking. Furthermore, the grafted PDLA chains preferably formed stable stereocomplex crystallites with the PLLA matrix, and the CNT self-networking resulted in the self-assembly of 3D continuous stereocomplex scaffold. It was demonstrated that the CNT-guided stereocomplex network endows polylactide-based nanocomposites with significantly improved mechanical strength, heat-resistance, and electrical conductivity at low CNT concentrations.

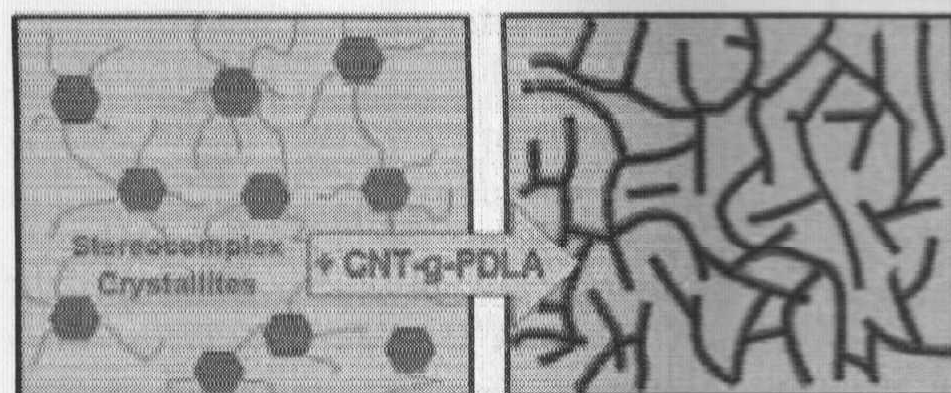


Fig. 1 Schematic diagrams of stereocomplex crystallite (Sc) structure in (a) PLLA/PDLA blends where some Scs may be bridged by polymer chains at high PDLA concentrations and (b) PLLA/CNT-g-PDLA mixtures where Sc forms along the CNT networks.

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### B22: Self-Assembly of Peptides into Nanotubes

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A short peptide, A<sub>6</sub>K, above a critical concentration is shown to form nanotubes [1]. Further increase in concentration results in a phase transition to first hexagonal then lamellar phase [2]. The local organization of peptide in the nanotube wall is found to be beta sheets organized in pairs that are two offset from each other [3]. Increase of temperature causes the nanotubes to dissolve and the mechanism is investigated using cryo-TEM. Using SAXS and cryo-TEM, formation of nanotubes by solid peptide dissolution and temperature quench is also investigated and the mechanism of formation and dissolution of nanotubes is revealed [4]. However, similar peptides that are slightly longer, A<sub>8</sub>K and A<sub>10</sub>K do not form nanotubes at any concentration, instead form fibrils [5]. This raises the question on self-assembly versus precipitation which will be discussed in this talk.

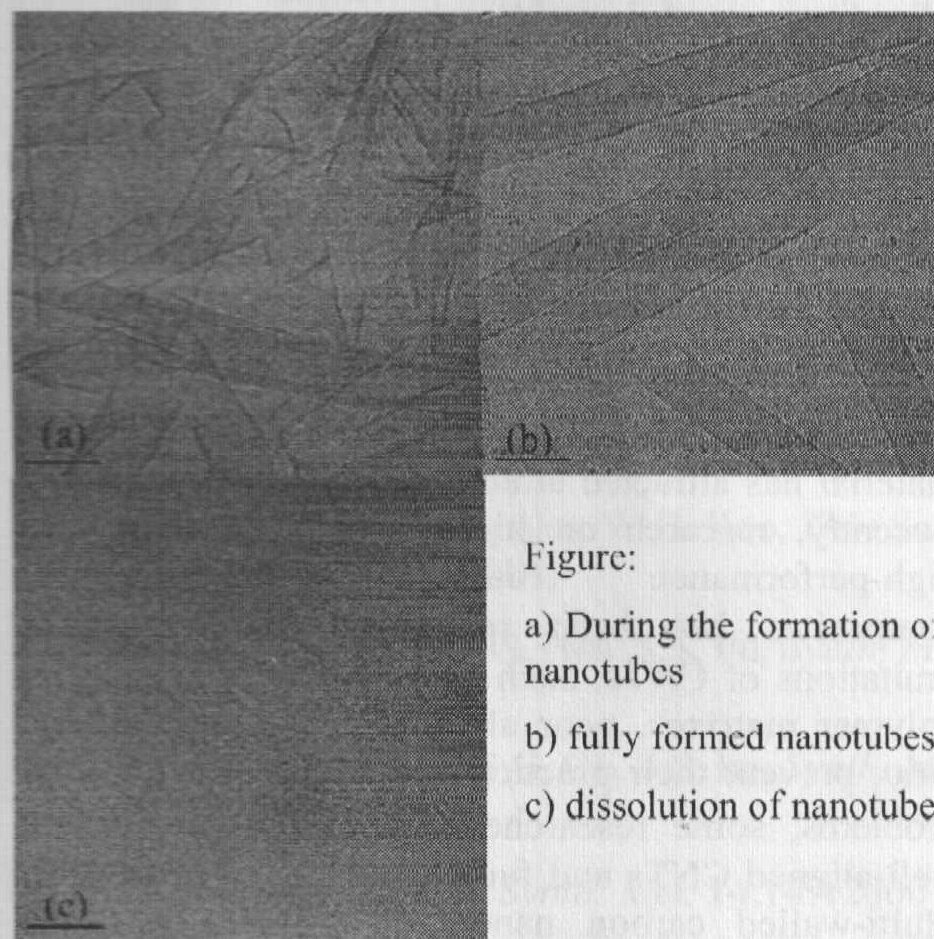


Figure:

- a) During the formation of nanotubes
- b) fully formed nanotubes
- c) dissolution of nanotubes

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### **B23: Enhanced Mechanical property of Aligned Carbon Nanotubes /Polymer composite**

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The development of CNTs as a reinforcement material has attracted attention in composite science. Recently, research on high-strength structural and high-performance functional CNT/polymer composites has been reported. However, some limitations of CNTs, such as their poor dispersity in polymer matrixes, poor alignment, and short aspect ratio, prevent their practical use. To overcome these problems, some researchers have been developing well-aligned CNTs and functionalizing CNT surface. Multi-walled carbon nanotubes (MWCNTs) were synthesized a simple and efficient synthesis method for producing vertically aligned long MWCNTs. Using these CNTs, well-aligned CNT sheets are produced by pulling it out from array. The synthesized CNT sheets have been functionalized by thermal treatment with various conditions. We have then observed experimentally that the interaction properties between CNTs surface and polymer can enhance the

tensile strength and elastic modulus of CNT/polymer composites.

### **B24: Thermo-mechanical properties of Carbon nanotubes and applications in thermal management**

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Carbon nanotubes (CNTs) are well-known nanomaterials with many excellent properties. Owing to their very high thermal conductivity (2000 W/m.K), high Young's modulus (950 GPa) and unique tensile strength (63 GPa), CNTs become one of the most suitable nano additives for fabricating heat conductive materials. In this work, we summary the obtained results on synthesis of heat conductive materials containing CNTs including thermal greases, nanoliquids and lubrication oils.

These synthesized heat conductive materials were applied in thermal management for high power electronic devices (CPU, LED) and internal combustion engines. The simulation and experimental results on thermal greases for Intel Pentium IV processor showed that the thermal conductivity of greases increases 1.4 times and saturation temperature of the CPU decreased about 5°C by using thermal grease containing 2 wt. % CNTs. We also successfully synthesized the nanoliquids containing CNTs based distilled water/ethylene glycol (DW/EG) and applied this nanoliquids in heat dissipation for Intel Core-i5 processor and 450 W Floodlight LED. The experimental results showed that the saturation temperature of the Intel Core-i5 processor and 450 W Floodlight LED decreased about 6°C and 3.5°C when using nanoliquids containing 1 g/l of CNTs volume concentration, respectively.

The CNTs was also utilized as additive material for synthesis of lubricating oils in order to improve the



thermal conductivity, heat dissipation efficiency and performance efficiency of engine. The experimental results show that the thermal conductivity of lubricating oils increase about 15%, the temperature of engine dropped 10°C, the fuel saving of engine was 15%, and the longevity of lubricating oil increased to 20,000 km by using 0.1% vol. CNTs in lubricating oils. All above results have confirmed the tremendous application potential of heat conductive materials containing CNTs in thermal management for high power electronic devices, internal combustion engines and other high-power machines.

### B25: Preparation and property of polyaniline nanocomposites containing TiO<sub>2</sub> nanoparticles and carbon nanotubes

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Rapid development in space technology, navigation, telecommunications, aircraft technology and rapid proliferation of electronic devices and wireless systems over past few decades has increased the vulnerability to electromagnetic interference (EMI) [1]. Conducting polymer plays an important role in technologies such as stealth, electrostatic charge dissipation and EMI interference shielding [2].

Nowadays, nanotubes or nanowires have attracted considerable attention because of their unique properties and promising potential applications in nanodevices [3-6]. As nanomaterial possessing moderate conductivity, magnetic and dielectric property, hexanoic acid (HA)-doped polyaniline (PANI) nanocomposites containing TiO<sub>2</sub> nanoparticles (dielectric filler) and carbon nanotubes, CNTs (magnetic fillers such as single-walled carbon nanotube, SWNT and multi-walled carbon nanotube, MWNT) were prepared by template free method. The PANI were characterized by UV, FTIR, X-ray diffraction (XRD), thermogravimetric (TGA) and scanning electron microscopy (SEM) analyses. Conductivity, magnetization, dielectric and microwave absorption properties of PANI were also investigated. The resulted nanorods/tubes as shown in SEM images clearly show that polymerization is proceeded in micelle/water interface through elongation. During template free method, TiO<sub>2</sub> and

CNT exist in the center of Ani/HA micelle. The nanocomposites prepared at 0 °C resulted large amount of nanorods/tubes (high heterogeneity) compared with 25 °C. The nanocomposites prepared at 0 °C posses higher permittivity and heterogeneity, hence will give rise to good microwave absorption property (>99.0 % power absorption) in frequency range of 10 – 13 GHz compared with 25 °C (Fig.1). The SEM images show that some of the TiO<sub>2</sub> and CNT enwrapped with PANI layer indicate TiO<sub>2</sub> and CNT are just packed underneath the PANI and never attacked by PANI. PANI/HA/TiO<sub>2</sub>/SWNT with 20% of SWNT exhibits the best microwave absorption property (~99.2% absorption) with reflection loss of -21.7 dB at 6 GHz due to its moderate conductivity (1.27 S/cm), magnetization ( $M_s = 1.01$  emu/g), highest  $\tan \delta$  and heterogeneity.

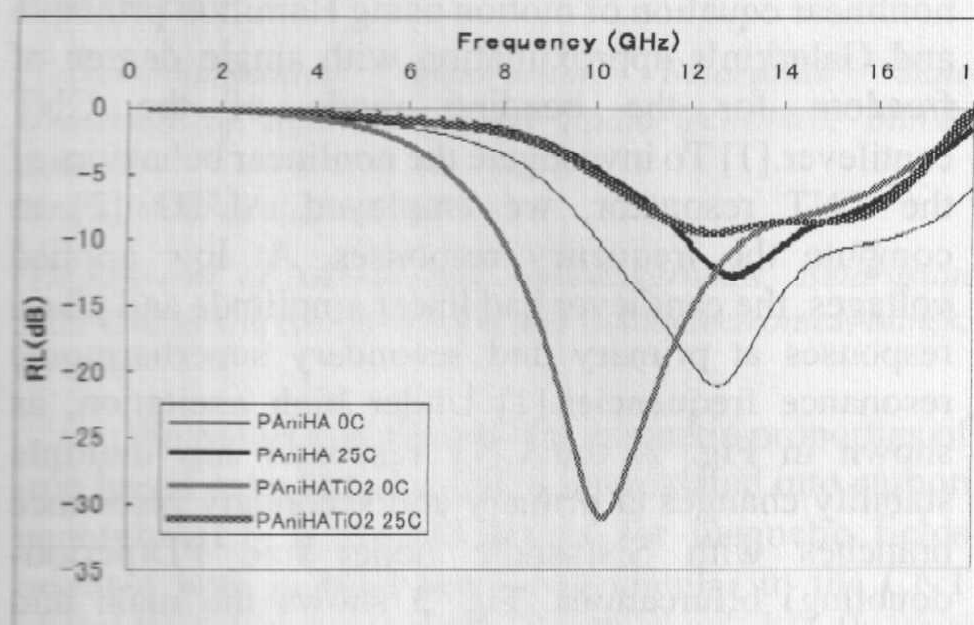


Fig.1. Reflection loss, RL of PANI/HA and PANI/HA/TiO<sub>2</sub> nanocomposites prepared at 0 °C and 25 °C.

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### B26: Nonlinear Mechanical Resonance of Cantilevered Carbon Nanotube with Electrostatic Excitation

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The electrostatic forces and intermolecular interactions based on Lennard-Jones potential model are considered between the single-walled CNT and a graphene surface. To accomplish the nonlinear dynamic analysis of resonating CNT cantilever, we established the differential equation model includes the geometric and inertial nonlinear terms due to the large deflection of the CNT vibration under electrostatic driving forces.[1] As a result, the CNT cantilever shows complex nonlinear responses due to the applied AC and DC voltages.

Fig. 1 shows an electrostatically actuated CNT resonator without any attachment. We derived the nonlinear equation of motion using Hamilton principle and Galerkin's approximation with single degree of freedom for the bending mode of the CNT cantilever.[1] To investigate the nonlinear behaviors of the CNT resonator, we employed AUTO [2] to compute the frequency responses. At low applied voltages, the cantilever had linear amplitude and phase responses at primary and secondary superharmonic resonance frequencies.[1] Under high excitation, as shown in Fig. 2, the CNT resonator has multiple stability changes at primary and secondary resonance branches with SN(saddle node) and PD(period-doubling) bifurcations. Fig. 3 shows the main and isolated solution branches with varying AC voltage. As increasing excitation voltage, it should be assumed that the isola is more developed and get closer to the main solution branch.

In summary, we predicted the nonlinear resonances of the CNT resonator under electrostatic excitation. The nano-resonator has complex behaviors such as softening effect, saddle-node or period doubling bifurcations as increasing the applied voltage. And the main and isolated solution branches were closer and coalesced as increasing harmonic voltage.

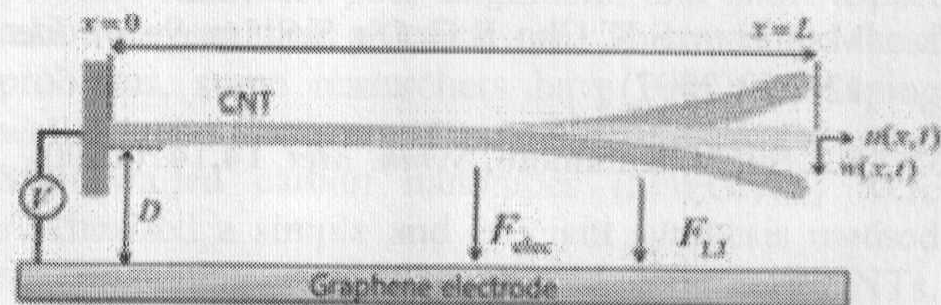


Fig. 1 Electrostatically actuated CNT resonator

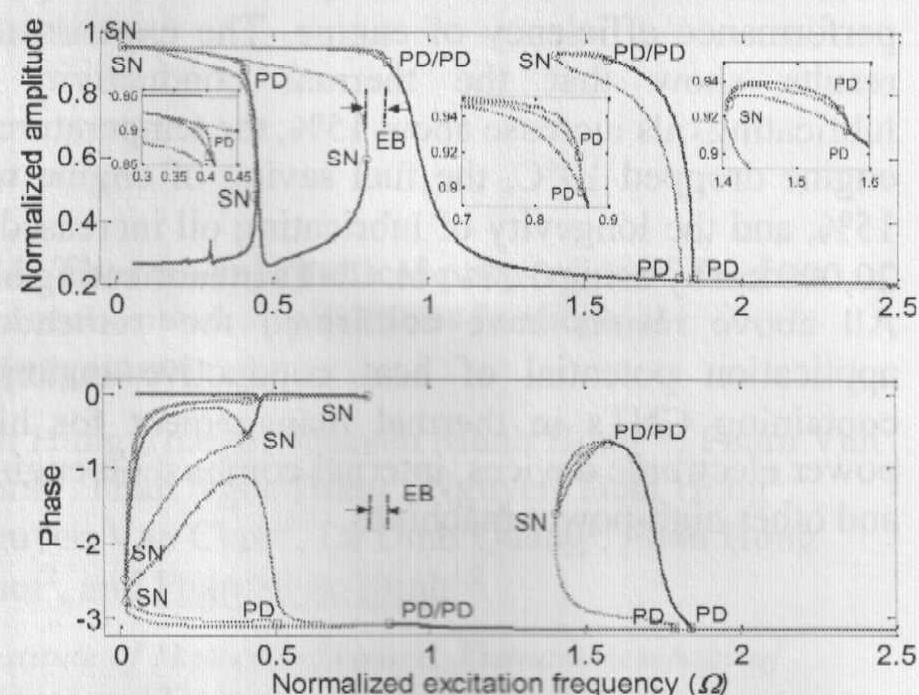


Fig. 2 Frequency and phase responses on DC voltage = 1.5 V and AC voltage = 0.2 V ( $Q=150$ ).

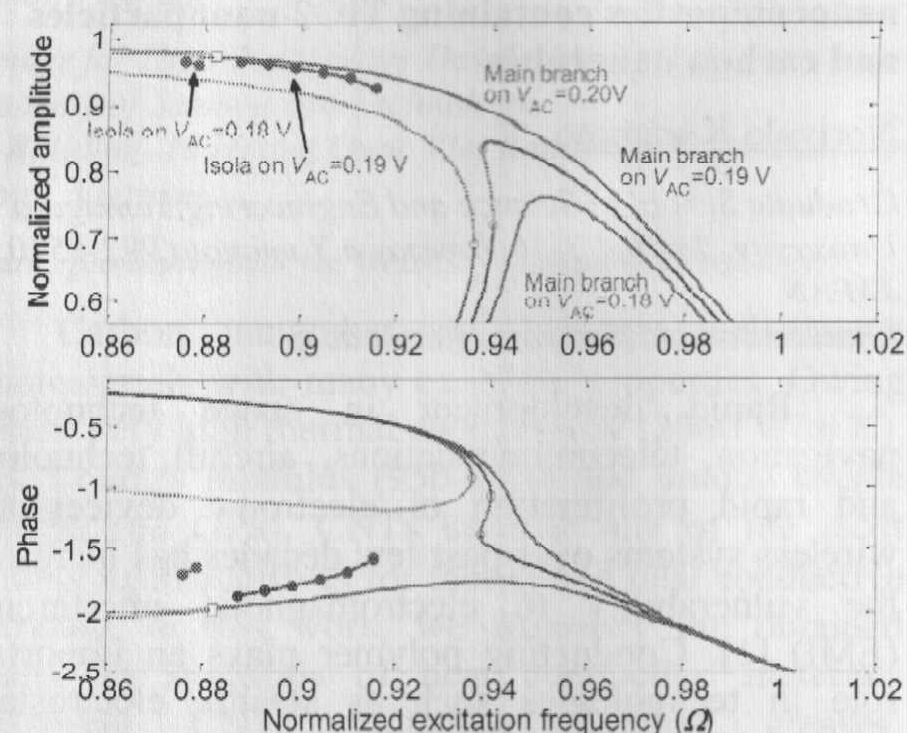


Fig. 3 Main and isolated branches for frequency and phase domain on DC voltage = 1.0 V and AC voltage variations ( $Q=20$ ). SN (o) is a saddle-node, and PD (□) is a period-doubling bifurcation

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## B27: Stiffness and conformation dependent polymer wrapping of SWCNT

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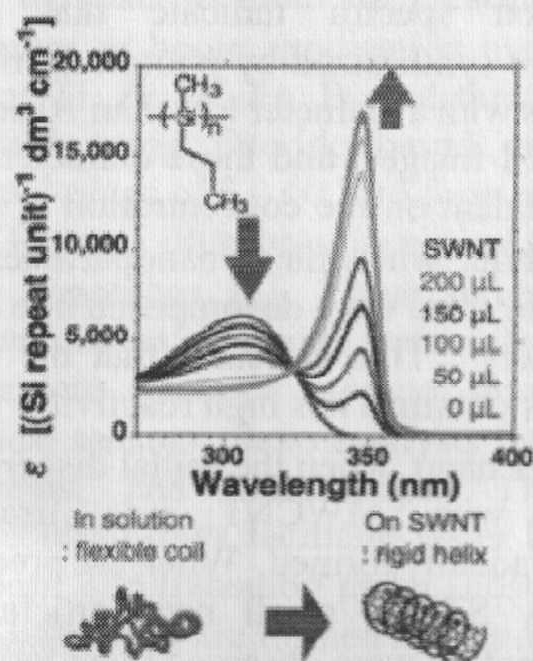


Figure 1. Changes in UV spectra of flexible PSi by addition of SWNT dispersion

Solubilization of single-walled carbon nanotubes (SWNTs) with various polymers has attracted a great deal of attention from functionalization / device application of SWNTs to fundamental polymer physics or surface chemistry. In this presentation, we would like to report a novel stiffness and conformation change of polydialkylsilane (PSi) along with polymer wrapping onto SWNT. Utilizing characteristic UV absorption of PSi originating from sigma-conjugation along Si main chain, we have elucidated changes in conformation of PSis during polymer wrapping (Figure 1). Consequently, we first demonstrated that CD-silent helical PSi with chiral side chains exhibited chiral induction along with its stiffness change when wrapped onto SWNT.

Among various types of chain-like polymers, polydialkylsilane (PSi) was used as one suitable model for elucidating the uniqueness of chain-like polymers on surfaces.<sup>1)2)</sup> This is because its controllable molecular length, polydispersity, stiffness, and terminal group by an adequate molecular design, a careful synthesis, and a precise purification, and highly luminescent chromophore due to Si-Si\* transition along the Si main chain. We will also show Time-resolved observation of chiral-index-selective wrapping on single-walled carbon nanotube with non-aromatic polysilane.<sup>4)</sup>

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## B28: Anisotropic Interaction of Ferromagnetic Nanoparticles Intercalated in Aligned Array of Carbon Nanotubes

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We report and discuss the magnetic properties of iron based nanoparticles (NPs) intercalated into carbon nanotube (CNT) aligned arrays for magnetic fields oriented both parallel and perpendicular to the CNT axes. Samples have been synthesized by floating catalyst chemical vapor deposition. They are characterized by HRTEM and XRD. A low continuous iron concentration in the gas mixture allows inserting selectively the iron nanoparticles particles inside the nanotubes. The NPs are mainly made up of iron carbide Fe<sub>3</sub>C with different crystallographic orientation. The NPs density distribution is directly related to the iron concentration in the feed solution.

We show that for the parallel field the interplay between the exchange coupling and magnetic anisotropy depends both on the NP content  $N_c$  and temperature  $T$ . For low  $N_c$  and  $T$  the magnetic anisotropy dominates [1]. Temperature increase leads to strengthening of the exchange interaction contribution. Moreover, analyzing the law of the approach to saturation [2] we have obtained evidence of the extended orientation order due to the coherent magnetic anisotropy at low  $T$  [3]. This magnetic order is strengthened by the CNT alignment. Increase in concentration of NPs destroys the coherent anisotropy [4]. For the perpendicular field the exchange interaction dominates in the whole studied temperature range (2–300K) independently on the  $N_c$  value. This is because



NPs belonging to different CNTs have to be considered in this case. Consequently, coherent anisotropy is destroyed due to loss of orientation of CNTs, and the exchange interaction is maintained by the indirect exchange via the conduction electrons of different CNTs, arbitrarily contacting each other. In addition, for the perpendicular field we have observed a crossover from two-dimensional to three-dimensional magnetic correlations with increasing temperature. Possible mechanisms of the observed effects are discussed paying special attention on the impact of the CNT medium on the interaction between ferromagnetic NPs.

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## **B29: Production and reactivity of oxidation-resistant metallic nanoparticles on carbon nanotubes**

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Copper nanoparticles have attracted much attention because they have a potential for substitution of precious and worth metal nanoparticles such as gold nanoparticles [1-2]. In fact, various synthesis methods have been studied, but they usually use radical and hazardous reagents such as hydrazine in order to reduce copper ions which are more difficult to reduce than noble metal ions. In addition, they are usually oxidized readily because of their high reactivity. In these points of view, it is important to establish the environmental-friendly synthesis method and to examine their reactivity.

Copper nanoparticles were synthesized by similar photoreduction method reported previously [3-4]. Copper acetate was dissolved in ethanol, and was mixed with powder of PVP or MWCNT. The mixed dispersion thus prepared was photoirradiated by Hg lamp. The obtained sample was characterized by

optical absorption, electron microscope, and X-ray diffractometer.

When the initial dispersion of copper acetate with PVP was irradiated by Hg lamp, its color was changed from light blue to deep red gradually. Corresponding optical absorption spectra indicate that copper nanoparticles were synthesized by photoreduction. In fact, nanoparticles with a diameter less than 10 nm were observed in STEM images, and these diameters were found to be dependent on the concentration of copper acetate. Meanwhile, when these nanoparticles were exposed to fresh air, they were decomposed into copper acetate immediately. This indicates that the copper nanoparticles thus obtained has high reactivity.

On the other hand, when the initial dispersion of copper acetate with MWCNT was irradiated, precipitate was gradually formed. When the precipitate was analyzed by STEM, small nanoparticles with similar size distribution were observed to be formed on MWCNTs. In addition, they were found to be composed of copper metal core covered with Cu<sub>2</sub>O thin layer by HRTEM observation. The existence of the Cu<sub>2</sub>O layer was also confirmed by XRD pattern. Furthermore, these nanoparticles were not decomposed by exposure to fresh air, and the XRD pattern was found to be unchanged for more than 2 months. This indicates that the synthesized copper nanoparticles are highly oxidation resistive because of the protection of the Cu<sub>2</sub>O layer for the metallic copper core.

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## **B30: Anodic Oxide Nanotubes for Energy Applications: Understanding Formation Mechanism and Defect Structures**

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Ordered arrays of vertically oriented metal oxide nanotubes have been prepared by a simple electrochemical route since 1996 [1]. The electrochemical route can either be an electrodeposition process using nanoporous aluminum oxide template as mold for creating the metal oxide nanotubes or be an anodization method. Pure metals such as Ti, Zr, W, Fe, Bi and their alloys have been anodized using fluoride based electrolytes in the potential range of 5 – 60 V to form nanotubular oxides [2-4]. Figure 1 illustrates the typical morphology of the oxide nanotubes [5]. These oxide nanotubes find applications as electrode materials for solar energy conversions, energy storage devices, improvised chemical sensors, photo catalysts for removal of toxic chemicals, and biomaterials. The ordered-oxide nanotubular arrays facilitate faster kinetics of charge transport. The transition metal substrate on which the oxide nanotubes are formed acts as a current collector. Therefore, an electrode manufacturing step, involving coating with a slurry of active material + conductive additives which is followed in the conventional process, could be avoided.

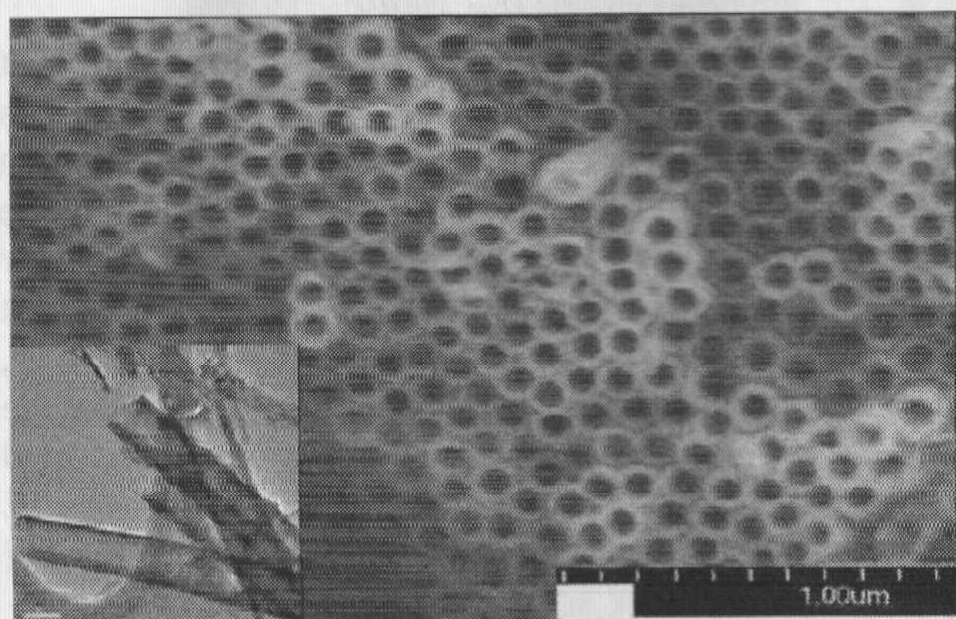


Fig. 1. Ti-Mn binary oxide nanotubes formed on to Ti-8Mn alloy. The inset shows the TEM image of the nanotubes.

Even though the preparation of anodic oxide nanotubes is a well-established process, the formation mechanism is not well understood. This presentation will give an overview of the proposed formation mechanisms reported in the literature and compare these with the surface perturbation theory that leads to pattern formation. It is postulated that the oxide growth stresses lead to surface perturbation and the surface energy component balances these growth stresses leading to a planar oxide layer. However, under specific anodic conditions (such as adsorption of ions, increased electric field, enhanced ionic flux due to surface curvature etc.), the surface energy is decreased which leads to enhanced surface perturbation and pattern formation. This presentation will elucidate the

role of defect structures such as oxygen vacancies on the nanotube formation, and energy storage behavior. The applications of  $\text{TiO}_2$ ,  $(\text{Ti}, \text{Mn})\text{O}_2$ , and  $\text{ZrO}_2\text{-WO}_3$  nanotubes for energy conversion and storage will be discussed with reference to defect concentrations and phase contents.

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### B31: Fabrication of CNT network and its application to GaN-based LEDs

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Indium tin oxide (ITO) has been used as a transparent conductive electrodes (TCEs) for various optoelectronic devices including light-emitting diodes (LEDs). However, indium's limited supply increases the price of ITO, and its rigid material's property limits its application to flexible devices. Furthermore, ITO has a large absorption in the ultraviolet (UV) region below 354 nm due to its narrow energy band gap of ~ 3.4 eV [1]. Therefore, much effort has been devoted to overcome these problems. Among those, nanoscale carbon materials such as carbon nanotube (CNT) and graphene have received a special attention owing to their outstanding electrical and optical properties.

In this study, we report the electrical and optical properties of single-walled carbon nanotube (SWNT) and reduced graphene oxide (RGO) films that exhibit high conductivity and transmittance in both visible and near-UV region [2]. Then, we propose a method for enhancing the electrical properties of SWNT and RGO films using a structure bridged with gold nanoparticles



(Au NPs) and a doping/chemical modification, as shown in Fig. 1. Finally, as an example of device application, we propose and fabricated GaN-based vertical LEDs with SWNT-networks (on the rough surface of n-GaN as a transparent conducting layer) not only to enhance the lateral current spreading but also external quantum efficiency via graded indexing and scattering effects, as shown in Fig. 2.

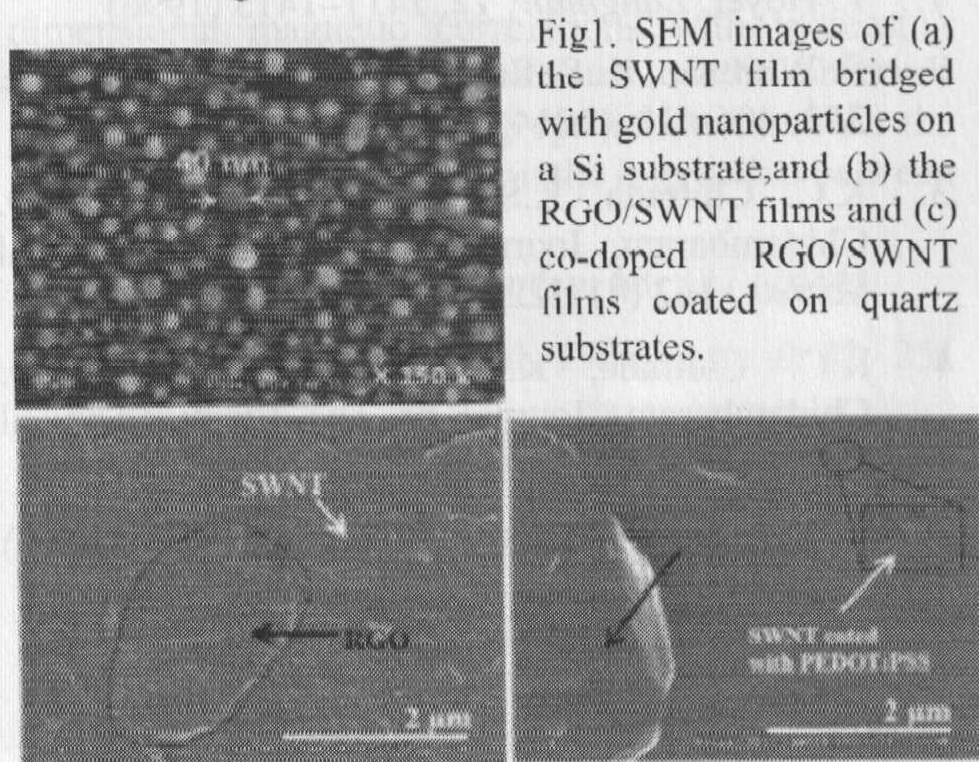


Fig1. SEM images of (a) the SWNT film bridged with gold nanoparticles on a Si substrate, and (b) the RGO/SWNT films and (c) co-doped RGO/SWNT films coated on quartz substrates.

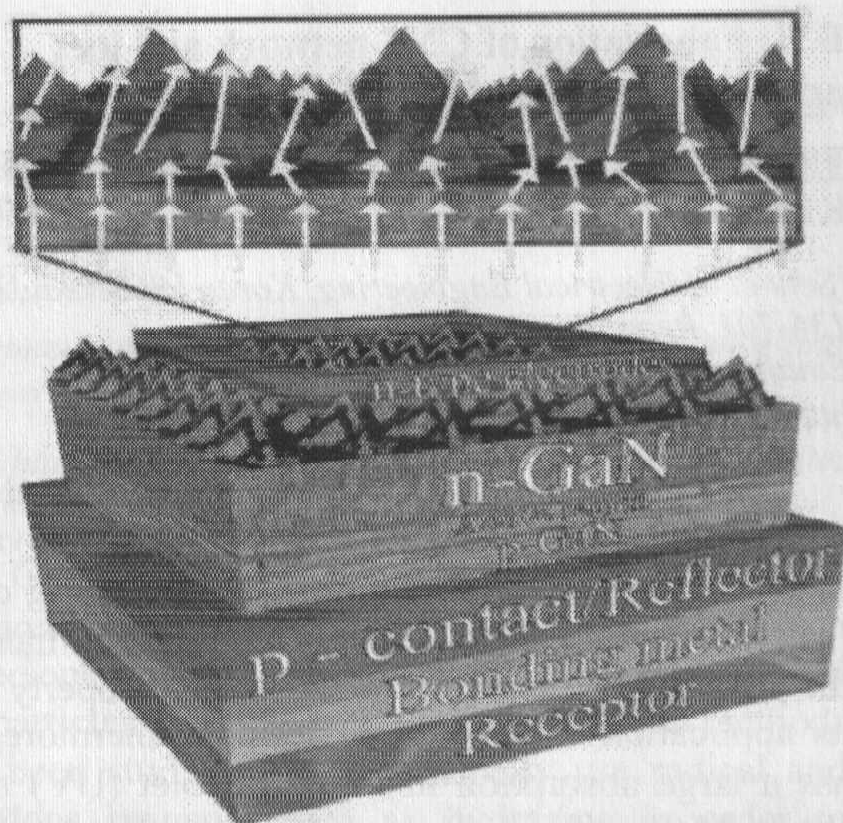


Fig. 2. GaN-based VLEDs incorporating the SWNTs as current spreading layers. (a) The schematic illustration of GaN-based vertical LEDs with surface roughened by wet etching and coated with ultra-thin SWNT-networks. The surface images for (b) 45° tilted-view and (c) top-view of the

ultra thin SWNT-networks formed on the roughened n-GaN surface of VLEDs.

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B32: TBA

### B33: Electrically Conductive and Thermally Insulative Polymer Nanocomposite Foams for Thermoelectric Applications

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Thermoelectric (TE) generators can harvest energy from waste heat generated by different sources (e.g., automobiles, electronic components, human bodies, etc.). Today's TE materials of choice are bismuth antimony telluride alloys; however, their scarcity, high cost, and toxicity for the environment have restricted their widespread uses. Recently, polymeric TE material systems [1] have become the subject of interest because they are cheaper, lighter, and easier to be processed; however, they have lower TE efficiency, which is commonly measured by the TE figure of merit ( $ZT$ ):

$$ZT = \frac{S^2 \sigma T}{k}$$

where  $S$  (in V/K) is the Seebeck coefficient,  $\sigma$  (in S/m) is the electrical conductivity,  $k$  (in W/mK) is the thermal conductivity, and  $T$  (in K) is the absolute measurement temperature.

A fundamental challenge to improve the efficiency of polymeric TE materials is the need to simultaneously improve their electrical conductivity and suppress their thermal conductivity. While embedding electrically conductive filler (e.g., carbon nanotubes and graphene) in polymer matrices would promote the electrical conductivity of the material system, it would also increase the thermal conductivity. In this context, this research aims to develop a novel strategy to tackle the aforementioned challenge. Using supercritical carbon dioxide as a physical foaming







**B35: Multi-dimensional carbon fusion bonding for supercapacitor**

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Carbon materials are strong candidate for energy storage as matters of weight and electron storages. T Advanced issues to be resolved arise for high energy storage with stability and efficiency. We suggest high performance electrode based on 3 dimensional carbon structures of graphenes with nano particles and nanorods. The most charging/discharging reaction of supercapacitor only occurs at surface of electorode. So, surface area has a significant effect in performance, the various pseudocapacitive materials were coated on the 3D carbon surface. . The influence of bath temperature on and electrochemical properties are studied. The morphology of the yields can be tailored only by controlling the reaction temperature of the bath; and has shown its prominence for the self-assembled growth leads transformation from hierarchical nano-brick, nano-leaf to nanobuds nanostructures. The prepared hybrid electrode was analyzed and optimized for efficiency.

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**B36: Carbon Nanotube Nanofluidics: from Fundamental to Applied Science**

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Owing to their simple chemistry and structure, controllable geometry, and a plethora of unusual yet exciting transport properties, carbon nanotubes (CNTs) have emerged as exceptional channels for fundamental nanofluidic studies, as well as building blocks for future fluidic devices that can outperform current technology in many applications. Leveraging the

unique fluidic properties of CNTs in advanced systems requires a full understanding of their physical origin [1] and the ability to assemble these nanochannels in optimal geometrical arrangements.

In this talk, we highlight experimental work performed in our laboratory directed toward: a) a fundamental understanding of the selectivity of these pores for electrolyte solutions under a pressure driving force; b) elucidating electric-field driven ion transport in a single CNT nanopore; c) the exploitation of CNT fast flow for the realization of ultrabreathable and protective CNT fabrics. For our studies, we used ceramic or polymeric membranes with well-aligned, a-few-nm wide CNTs as only through-pores. We provide evidences of a pH-tunable ion selectivity in narrow CNT pores that is dominated by electrostatic interactions between carboxylic groups at the CNT tips and the ions in solution. [2-3] With single-pore ionic conductance measurements, we reveal giant ionic currents in CNT pores that follow an unusual power-law concentration dependence. Finally, we show that flexible CNT membranes (Figure 1) provide diffusion-driven water-vapor transport rates that are comparable to or exceeding state-of-art breathable fabrics at all relative humidities even if the moisture conductive pores are only a-few-nm wide and the membrane porosity is <5%. Moreover, these tiny pores enable simultaneous passive protection from biological threats by size exclusion. [4]

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-665307

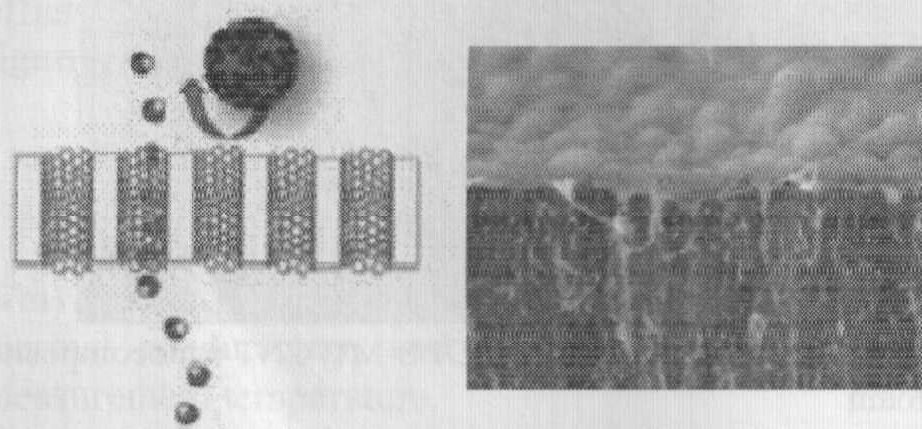


Fig1. Schematic representation of an ultrabreathable CNT membrane rejecting a viral particle (left), and SEM image of the cross-section of the corresponding CNT-polymer composite (right).

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### C01: Graphene nanosystems and low-dimensional Chern-Simons topological insulators

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A graphene nanoribbon is a good candidate for a (1+1) Chern-Simons topological insulator since it obeys particle-hole symmetry. We show that in a finite semiconducting armchair ribbon, which has two zigzag edges and two armchair edges, a (1+1) Chern-Simons topological insulator is indeed realized as the length of the armchair edges becomes large in comparison to that of the zigzag edges. But only a quasi-topological insulator is formed in a metallic armchair ribbon with a pseudogap. In such systems a zigzag edge acts like a domain wall, through which the polarization changes from 0 to  $e/2$ , forming a fractional charge of one-half. When the lengths of the zigzag edges and the armchair edges are comparable a rectangular graphene sheet (RGS) is realized, which also possesses particle-hole symmetry. We show that it is a (0+1) Chern-Simons topological insulator. We find that the cyclic Berry phase of states of a RGS is quantized as  $\pi$  or 0 (mod  $2\pi$ ), and that the Berry phases of the particle-hole conjugate states are equal each other. By applying the Atiyah-Singer index theorem to a long rectangular ribbon and a RGS we find that the lower bound on the number of nearly zero energy end states is approximately proportional to the length of the zigzag edges. However, there is a correction to this index theorem due to the effects beyond the effective mass approximation.

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## C02: Graphene - Nano-electromechanical system switches and van der Waals (vdW) interaction controlled sensing of CO<sub>2</sub>

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Graphene, as a monolayer of graphite, has an ultra-high Young's modulus of  $\sim 1$  TPa, which makes it a promising candidate for Nano-Electromechanical (NEM) devices. The graphene NEM switches is

expected to show minimized electrical leakage, sharp switching response, low actuation voltage, and high on/off ratio. A simple bottom-up procedure using a polymer sacrificial spacer is utilized to fabricate graphene electromechanical contact switch devices. Low pull-in voltage of below 5 V is achieved with good consistency [1], which is compatible with the conventional complementary metal-oxide-semiconductor circuit requirements. In addition, the formation of carbon-gold bonds at the contact position is proposed as another important mechanism for the irreversible switch other than the well-known irreversible static friction.

In order to overcome the stiction issue and realize the repetitive switching operations, natural chromium oxide formed in the chromium electrode was exploited. Towards this direction, we report double-clamped beam and cantilever graphene nanoelectromechanical switches with local top actuation electrode. The low pull-in voltage below 5 V was realized in both of the switches (Fig. 1(a)). As a consequence of the naturally formed chromium oxide at the contact interface to prevent the formation of chemical bonds between graphene and metal electrode, the reversible switching operation was achieved.

Owing to the high-quality crystal lattice along with its 2D structure, graphene exhibits an extremely suppressed electrical noise, making it possible to realize high sensitivity sensor. With the physisorbed CO<sub>2</sub> molecules - graphene vdW complexes, we have discovered the tunability of the vdW interaction at external electric fields. The field-dependent charge transfer in CO<sub>2</sub>-graphene complex was unveiled with associated changes in the equilibrium CO<sub>2</sub>-graphene distance and the O-C-O bonding angle. By reversing the substrate bias polarity, the charge transfer direction also switched, signifying the role of physisorbed CO<sub>2</sub> molecules can be altered electrically between donor

and acceptor (Fig. 1(b)). The range of electrical tunability is a unique feature for each type of molecule [2].

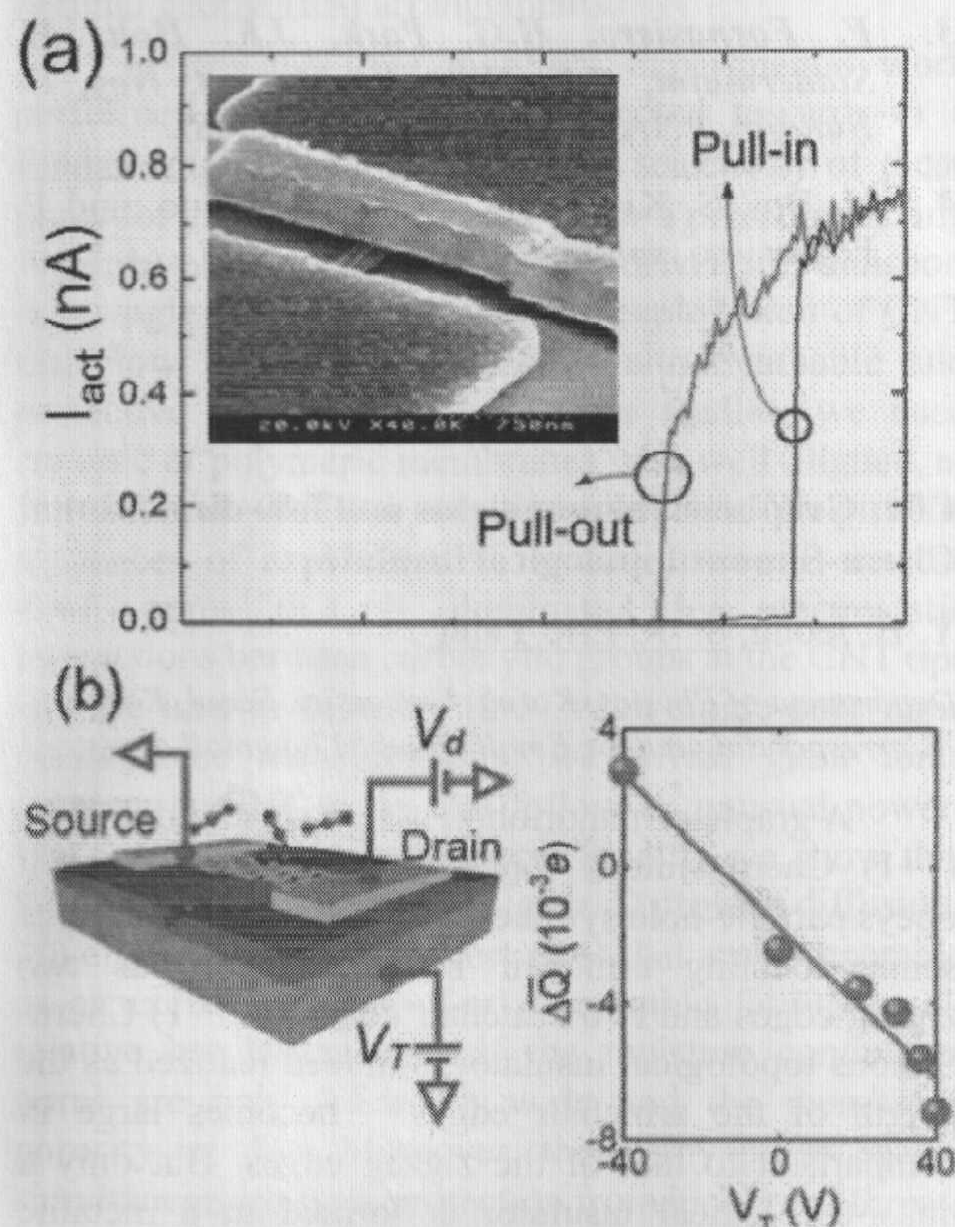


Fig. 1 (a) Switching performance of the double-clamped monolayer graphene nanoribbon (Inset: SEM image of the suspended graphene switch). (b) Schematic of the graphene sensor measurement configuration and plot of the charge transfer for various tuning voltages.

### Acknowledgement:

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**C03: Stretchable, Transparent Electrodes using hybrid structures of 1D-2D Nanomaterials for Wearable Electronics**Jang-Ung Park<sup>1</sup>

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Up to now, indium tin oxide (ITO) deposited by sputtering process is used as the main TCE substance. Although the ITO exhibits excellent properties of low sheet resistance ( $\sim 30 \text{ Ohm/sq}$ ) and high transparency ( $\sim 90 \%$ ), its fragility limits many potential applications in flexible and stretchable electronics. Several alternative materials to ITO, including conducting polymers, carbon nanotubes, graphene, and metal nanowires, have been studied as candidates of the flexible and stretchable TCEs. Although many of these candidates exhibit good mechanical flexibility and stretchability, none shows significantly higher conductivity and transparency together, compared to ITO.

Here, we present a simple fabrication process of high-performance, stretchable TCEs based on the metal nanotrough which have long and continuous random web geometries, constituting hybrid with 2D material graphene. These TCEs show superb electric conductivity ( $\sim 1 \text{ ohm/sq}$ ) with high transparency ( $\sim 91\%$ ) as well as excellent flexibility and stretchability. Hybrid transparent electrode shows very stable electrical properties even under  $50 \mu\text{m}$  radius bending and 80% stretching (sheet resistance changed less than 20%). Also, hybrid film shows great uniformity, verified by the reduced standard deviation of sheet resistance by one-tenth compare to that of metal nanofiber only. Based on these outstanding mechanical and electrical properties, we demonstrate a transparent and flexible thin film transistor (TFT) backplane, composed of the AgNW-graphene hybrid film, zirconium aluminum oxide, indium oxide, and metal nanotrough-graphene hybrid film. Fabricated oxide TFT shows mobility as high as  $100 \text{ cm}^2/\text{V}\cdot\text{s}$  and transparency of  $\sim 90\%$ . TFT backplane can be transferred to various substrates such as a leaf, glass cup, glass, and human skin. We believe these TCEs based on the nanostructures present a promising strategy toward flexible and wearable electronics beyond the limits of conventional ITO.

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**C04: Modified Epitaxial Graphene on SiC for Selective and Highly Sensitive Gas Sensors**Jens Eriksson<sup>1</sup>, R. Yakimova<sup>1</sup>, A. Lloyd-Spetz<sup>1</sup>

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We report on surface modifications of epitaxial graphene on SiC (EG/SiC) with metal-oxide (MOx) nanoparticles (NPs) and monolayers, formed by reproducible thin film deposition techniques, and their effect on the electronic properties of the graphene and on gas interactions at the graphene surface. The scope is to exploit the sensing properties of MOx materials for selectivity tuning while utilizing the unique electronic properties of graphene as an ultra-sensitive transducer.

We have previously found that monolayer graphene is crucial for optimum gas sensitivity [1]. This highlights the importance of achieving well-controlled uniform single-layer graphene growth. To that end, we have shown [2] that the graphene thickness uniformity can be significantly tuned by careful control of the EG/SiC morphology.

Chemiresistor sensors based on EG/SiC, decorated with Au, Pt,  $\text{TiO}_2$  and  $\text{Fe}_3\text{O}_4$  core-shell NPs, were tested towards parts per million (ppm) down to low parts per billion (ppb) concentrations of hazardous volatile organic compounds (VOCs), e.g.  $\text{CH}_2\text{O}$  and  $\text{C}_6\text{H}_6$ , as well as common pollutants like  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{CO}$ , and  $\text{NH}_3$ , which are all gases relevant for air quality monitoring and control. While pristine EG/SiC showed no response to the tested VOCs, it was found that decoration with  $\text{TiO}_2$  or  $\text{Fe}_3\text{O}_4$  NPs can yield selective detection of both  $\text{CH}_2\text{O}$  and  $\text{C}_6\text{H}_6$ . The effect of decoration on the sensor performance strongly depends on the choice, thickness, surface coverage, and size of the NPs. Decoration with nanoporous (2-3 nm) Au improved the detection limit and selectivity for  $\text{NO}_2$  [3]. Decoration with  $\text{TiO}_2$  NPs allowed detecting low ppb levels of formaldehyde and benzene, where the effect



on the sensor performance depends on the diameter and surface coverage of the deposited  $\text{TiO}_2$  NPs. Graphene decorated with monodispersed  $\text{Fe}_3\text{O}_4$  NPs showed an even larger sensitivity to formaldehyde (Fig. 1a) and benzene (Figs. 1b and 1c) compared to EG- $\text{TiO}_2$  NP hybrids.

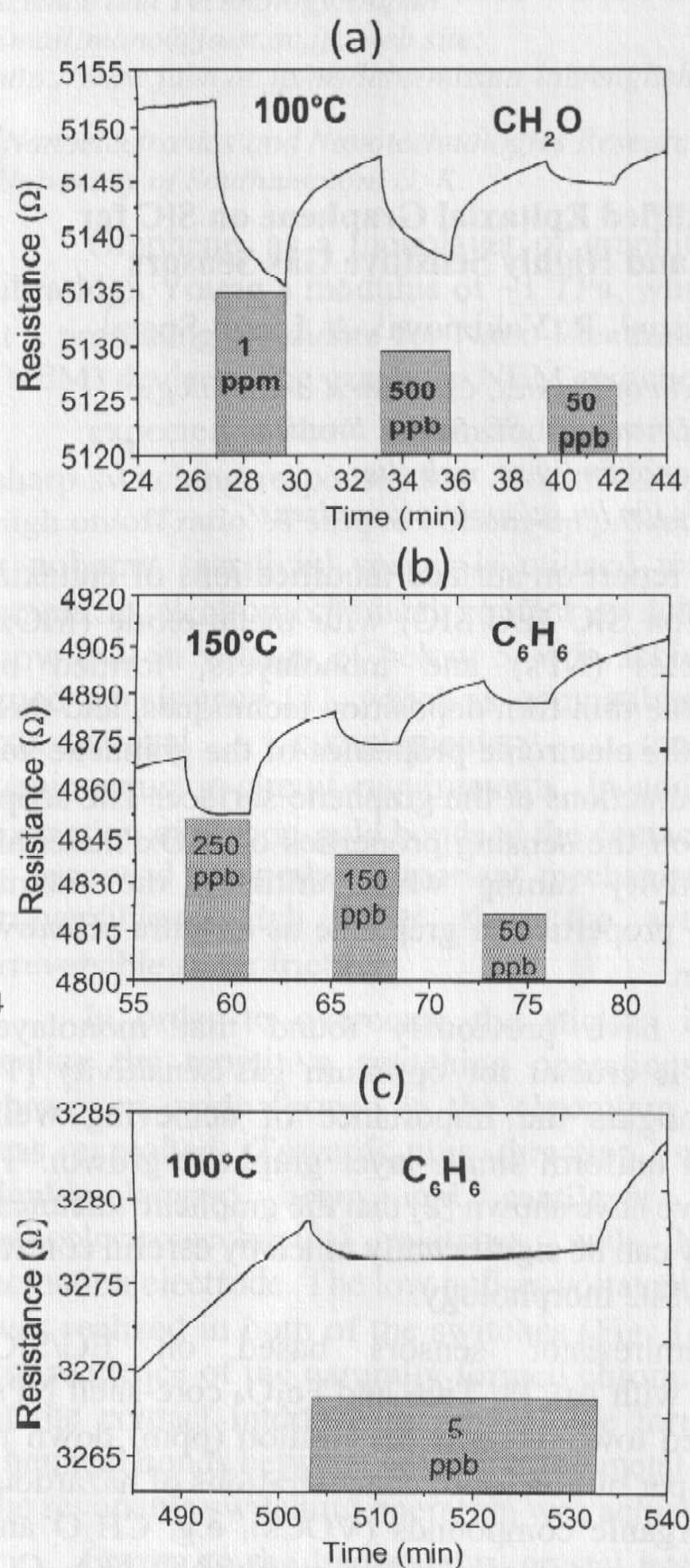


Fig1. Response of a EG/SiC sensor decorated with FeO core-shell NPs ( $\approx 60$  nm in diameter) to  $\text{CH}_2\text{O}$  concentrations from 1 ppm to 50 ppb (a) and to  $\text{C}_6\text{H}_6$  concentrations in the range 250-50 ppb (b) and 5 ppb (c).

The results show that graphene decoration can be an effective strategy for tuning the sensor performance in the scope of ultra-sensitive detection of toxic air pollutants.

The presentation will also include results on

other monolayer gas sensing layers like iron oxide on top of platinum on SiC, which offer additional possibilities like operation at high temperature and in harsh conditions, while maintaining all the promises of 2D materials as extremely sensitive transducers.

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### C05: Applications of Nanotechnology in Fuel Energy and Propulsion

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The modern advent of nano- science/technology is usually marked with a lecture delivered by the Noble laureate Richard Feynman in 1959 titled "There is Plenty of Room at the Bottom". Since then, there have been tremendous progresses in a large number of directions using products manufactured, and information learned, from nanoscale materials. Nano-science is truly a multidisciplinary subject which has penetrated into a large number of other areas/applications such as medicine, pharmaceutical, dentistry, textile, sports, automotive, computers, and energy, to name a few. In this presentation, a select number of applications of knowledge learned at the nanosized range are briefly discussed in the context of fossil fuel production and propulsion. The aim is to demonstrate the great potential of nanostructured materials in petroleum refining industry, contributing towards efficient production of fuels and thereby of different forms of energies. In particular, the catalytic role they play is of paramount importance, especially considering that energy producers are switching to ever-heavier fossil feedstocks (heavy oil, tar sands, shale oil, and coal) while the supply of light petroleum feedstock (high in hydrogen and low in sulfur and nitrogen) is rapidly depleting. Applications of nanostructured materials in naphtha reforming, hydrotreating (or hydrodesulfurization), conversion of syngas (Water- gas shift and Fisher-tropsch), and use of graphene/carbon-nanotubes in ignition, combustion and propulsion are presented.



**C06: Electron transport through graphene-BN-graphene heterostructures**Supeng Ge<sup>1</sup>, K. M. Masum Habib<sup>2</sup>, and Roger K. Lake<sup>2</sup><sup>1</sup>Department of Physics and Astronomy, University of California, Riverside, CA, USA<sup>2</sup>Department of Electrical and Computer Engineering, University of California, Riverside, CA, USAEmail:rlake@ece.ucr.edu, web site: <http://latte.ece.ucr.edu>

There have been a number of recent studies of graphene / boron-nitride / graphene devices that exhibit negative differential resistance (NDR). Theoretical analysis finds that such devices could oscillate at frequencies up to several hundred GHz [1]. The NDR arises from the line-up of the source and drain graphene Dirac cones combined with the conservation of in-plane momentum. While theoretical attention has been given to the misorientation of the graphene layers in the source and drain and the resulting misalignment of the Dirac cones, there has not yet been a study of the effect of the misalignment of the boron-nitride (BN) layer on the tunneling and its affect on the NDR. In the theoretical treatments, the misorientation of the BN layer has only been treated within a small angle approximation. The misorientation of two graphene layers can have a dramatic effect on the graphene-graphene interlayer electron transport. This motivates us to consider the effect of the BN alignment on the interlayer source-drain transport in G/BN/G devices.

To focus solely on the effect of the BN misalignment, we consider a system of two aligned graphene layers serving as the source and the drain separated by one or more AB stacked layers of h-BN that are misoriented with respect to the graphene. An illustration of such a system is shown in Fig. 1. The misorientation of the BN with respect to the graphene can have several possible effects. (a) It can alter the transverse momentum conservation and thus degrade the NDR. (b) It can alter the potential barrier seen by the electrons at the K points in the graphene, and thus alter the magnitude of the tunneling current. (c) As in misoriented graphene on graphene, it can result in destructive quantum interference that reduces the current. To analyse the source-drain transport, we employ a tight binding model for the Hamiltonian and a non-equilibrium Green function (NEGF) approach for the transport.

We find that the resistance monotonically increases as the BN is rotated from 0 to 30°. The overall change in resistance depends on the thickness of the BN layer. For a single monolayer, the resistance

increases by one to two orders of magnitude depending on the position of the Fermi level. For 3 monolayers the increase varies from 3 to 4 orders of magnitude. The change in resistance is well explained by effect (b). As the BN is rotated, the effective BN bandgap seen by an electron at the K-point in the graphene monotonically increases as the rotation angle increases from 0 to 30°. Plotting the current versus this effective BN bandgap shows an exponential relationship, as one would expect. This appears to be the dominant mechanism governing the current flow resulting from the misalignment of the BN. The BN rotation does not degrade the NDR or the peak-to-valley current ratios. Its primary effect is to reduce the overall magnitude of the current (by the same order of magnitudes as discussed above) while retaining all of the features of the I-V curves. Thus, the misorientation of the BN does not significantly effect the transverse momentum conservation required for NDR, but only the current magnitude, which is required for high frequency operation.

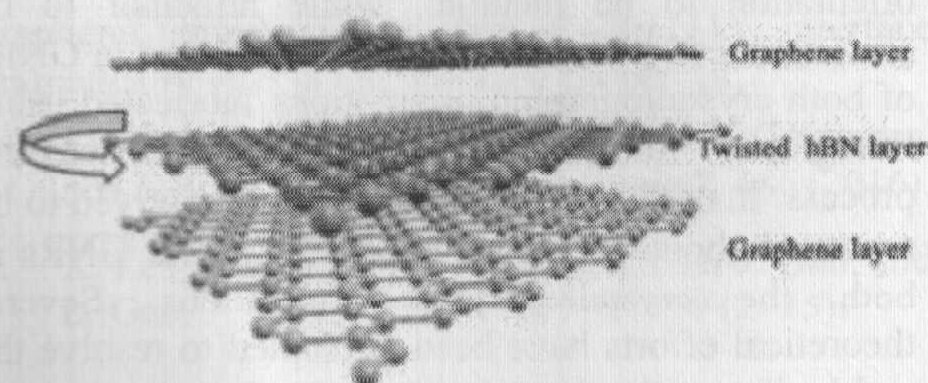


Fig. 1. Graphene / boron-nitride / graphene heterostructure. The top and bottom layers are aligned graphene. The middle boron-nitride layer is rotated with respect to the graphene layers.

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**C07: Edge configurational effect on band gaps in Graphene nanoribbons**Deepika<sup>1</sup>, T.J. Dhillip Kumar<sup>2</sup>, Alok Shukla<sup>3</sup>, Rakesh Kumar<sup>1\*</sup><sup>1</sup> Department of Physics, Indian Institute of Technology Ropar, Rupnagar 140001, INDIA<sup>2</sup> Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, INDIA



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Graphene is a zero band gap material, has been known to the scientific community for a long time even before its discovery in 2004. Graphene shows extraordinary electrical and other physical properties far better than that of being extensively used Silicon in the semiconductor industry. Therefore, Graphene is being seen as a material capable to replace silicon once the related technology saturates. Zero band gap of Graphene is the biggest roadblock for its electronic applications. Out of all the possible ways, how to open a band gap in Graphene; the best way to open a band gap is by quantum confinement of the charge carriers by fabricating it into Graphene nanoribbons (GNRs). *ab initio* calculations carried so far using Density Functional Theory (DFT) show that crystallographic edges in addition to the width of GNRs play a crucial role in the band gap formation. Theoretical calculations predict GNRs of zigzag crystallographic orientation to be metallic, while armchair to be semiconducting. But band gaps are observed in GNRs of both crystallographic orientations fabricated using lithography followed by oxygen plasma etching process. In addition, the band gaps are observed to be scattered about an average fitting curve for GNRs in both the crystallographic orientations. Several theoretical efforts have been attempted to resolve the ambiguity with the experiments, but have been insufficient.

In the talk, we put forward a resolution to the prolonged band gap ambiguity between theory and experiments of fabricated GNRs on the basis of edge configurations [1]. Our band structure calculations using density functional theory are performed on oxygen passivated GNRs supercells of customized edge configurations without disturbing the inherent  $sp^2$  hybridization of the carbon atoms. Direct band gaps are observed for both zigzag and armchair GNRs, consistent with the experimental reports. In addition, band gap values of GNRs scattered about an average value curve for a given crystallographic orientation are correlated with their width on basis of the edge configurations elucidates the band gaps in the fabricated GNRs. We remark that edge configurations of GNRs significantly contribute to band gap formation in addition to its width for a given crystallographic orientation, and it would play a crucial role in band gap engineering of GNRs for future research works on fabrication of nanoelectronic devices.

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#### **C08: Van der Waals stacks of few-layer h-AlN with graphene: an ab-initio study of structural, interaction and electronic properties**

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Since the start of its intense research in the late 1980's, group III nitrides, including AlN, GaN, InN, and their alloys, has become one of the most extensively studied and most widely applied classes of semiconductor materials for the development of short wavelengths light emitting diodes (LEDs) and lasers (2014 Nobel Prize in Physics). Group III nitrides naturally crystalize in the wurtzite (wz) structure represented by two interpenetrating hexagonal sublattices of group III atoms and nitrogen atoms, respectively.

Recently, graphite-like hexagonal AlN (h-AlN) multilayers have been experimentally manifested [1] and theoretically modeled [2]. The development of any functional electronics applications of h-AlN would most certainly require its integration with other layered materials, particularly graphene.

In our most recent work [3], by employing vdW-corrected density functional theory calculations, we investigate structure, interaction energy, and electronic properties of van der Waals stacking sequences of few-layer h-AlN with graphene (Figure 1). We find that the presence of a substrate such as graphene induces enough interlayer charge separation in h-AlN, favoring a graphite-like stacking formation. We also find that the interface dipole, calculated per unit cell of the stacks, tends to increase with the number of stacked layers of h-AlN and graphene.



In this presentation, we'll emphasize our encouraging theoretical findings on van der Waals stacks of few-layer h-AlN with graphene in the context of the vast competences on growth of III-Nitrides as well as on theoretical modelling of low-dimensional and layered material systems beyond graphene available in our group at Linköping University in Sweden.

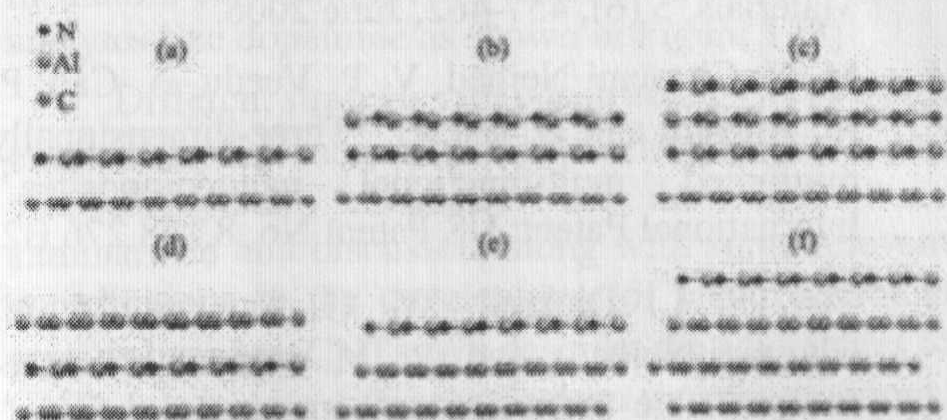


Fig. 1 Examples of stacking configurations of few-layer h-AlN and graphene.

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### C09: Scanning Tunneling Microscopy Studies of Hydrogen Desorption from Graphene and Transformation of C<sub>60</sub> into Graphene

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Atomic-scale investigation of the phenomena in graphene-related materials is crucial for the practical applications of graphene. Scanning tunneling microscopy (STM) is a unique and powerful technique to detect the structural, electronic, chemical and other properties of materials on the atomic scale. In this talk, I will discuss our recent STM studies of the hydrogen desorption from graphene as well as the transformation of C<sub>60</sub> into graphene. First, we investigated electron-

stimulated desorption of hydrogen from the graphene/SiC(0001) surface at room temperature.[1] Two different desorption processes were observed. We also found that the curvature of graphene dramatically affects hydrogen desorption. Second, we investigated the adsorption, electronic structure, and thermodynamics of C<sub>60</sub> molecules on Ir(111) and graphene/Ir(111) surfaces.[2] We found that C<sub>60</sub> interacts strongly with the Ir(111) surface, leading to a spontaneous formation of graphene on the Ir(111) surface at elevated temperatures. The introduction of a

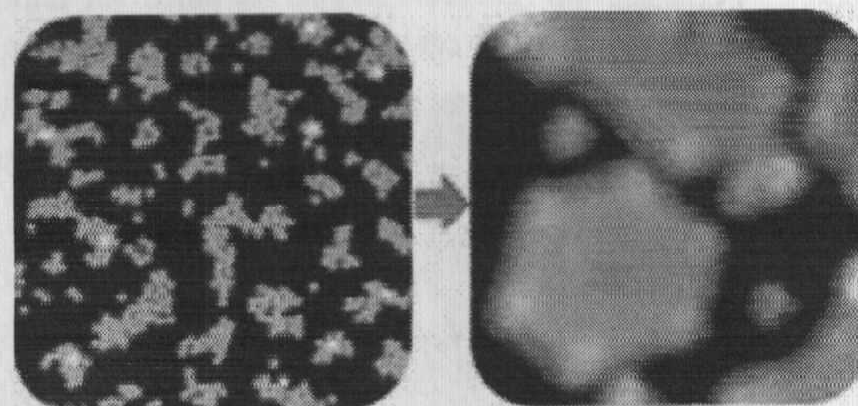


Fig. 1 The transformation of C<sub>60</sub> into graphene on the Ir(111) surface.

graphene interlayer at the C<sub>60</sub>/Ir(111) interface dramatically affects the interface properties.

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### C10: Application of Nanotube/Nanotechnology in Structures and Renewable Energy Productions and Storage Devices

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This paper presents a summary review on the applications of nanotubes/nanotechnology in the manufacturing of renewable energy production and storage devices. The use of carbon nanotubes (CNTs) and graphene nanosheets (GNSs) to improve the performance and durability of wind turbine and wave rotor blades will be reviewed. While GNS are primary used for the performance enhancement of the resin system to manufacture Nanoresins, CNT- Nanoforests and Nanofilms are used to improve the performance of fiber systems in a high-performance Nanocomposites.

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Next, the use of CNTs and GNSs in the manufacturing of other renewable energy production devices; such as, proton exchange membrane fuel cells (PEMFCs) and polymer solar cells as well as renewable energy storage devices; such as, batteries and supercapacitors to improve their performances, efficiencies, reliability, and durability while reducing their costs, weights, and sizes will be reviewed.

**Keywords**—Manufacturing, Nanotechnology, Carbon Nanotubes, Graphene Nanosheets, Renewable Energy Production Devices, Renewable Energy Storage Devices.

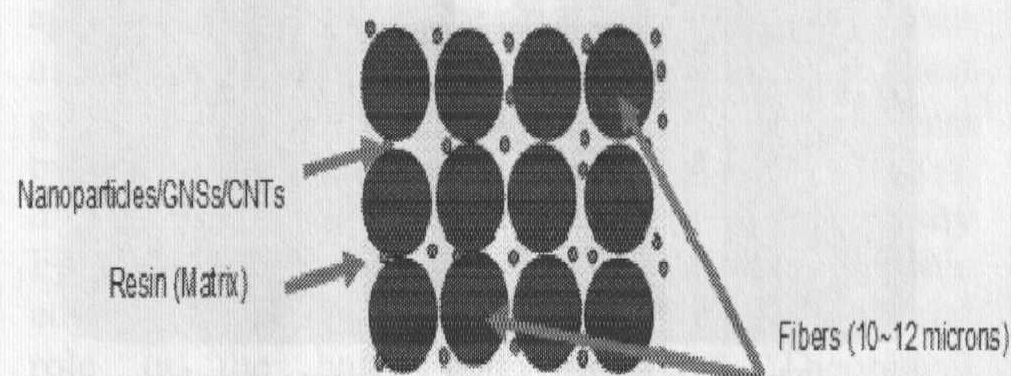


Figure 1 Inclusion of nanomaterials in resin systems [1-3].

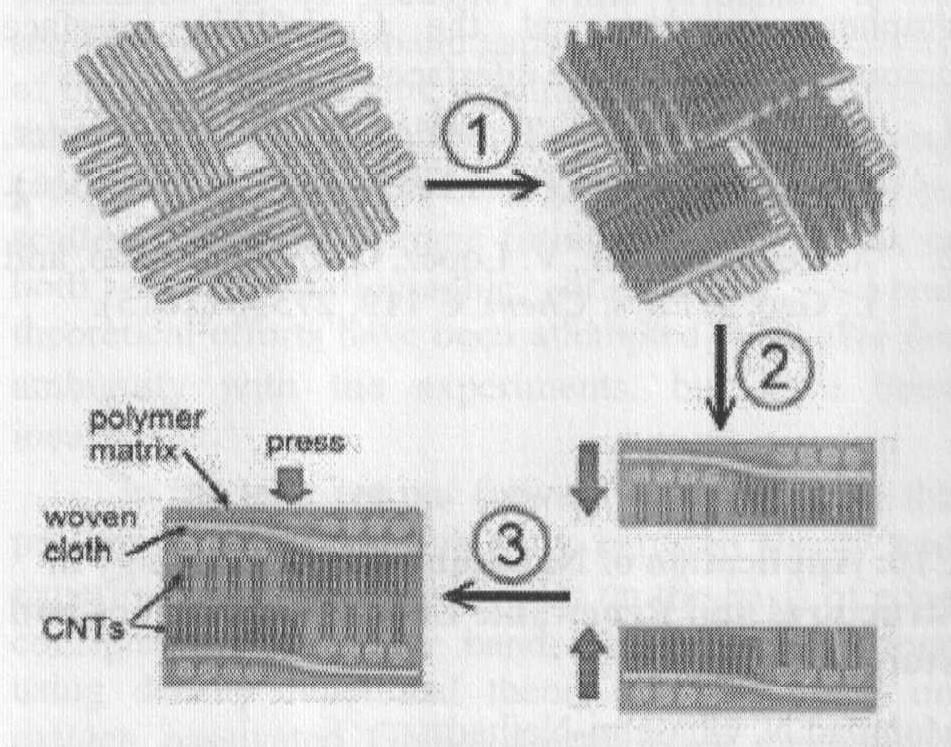


Fig2. Direct growth of CNTs on fibers [4-7].

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#### C11: Analytical applications of carbon nanotubes based electrochemical sensors

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Advances in nanofabrication of sensing interfaces are one major area where nanotechnology has dramatically impacted on electrochemical sensor research. An overview of analytical development demonstrates that electrochemical sensors represent the most rapidly growing class of chemical sensors. The application of carbon nanotubes (CNTs) most widely employed so far has been the construction of various detection devices, such as gas sensors, electrochemical detectors and biosensors with immobilized biomolecules. Their application in voltammetric methods is especially favorable, but they are also employed for sorption of different analytes and in electrochemical stripping methods. We mainly focused on voltammetric sensors.

With regards to fabricating sensing interfaces the rise of chemically modified layers has been particularly important in giving molecular level control over the fabrication of the sensing interface. Using chemical functionalities has resulted in better performing sensors



offering also new opportunities in developing new types of transduction mechanisms in sensors which are more sensitive and selective. Especially large number of applications can be found in the literature on applications of CNTs as electrode materials or modifiers of conventional working electrodes in analytical voltammetry.[1,2] Carbon nanotubes modified electrodes employing immobilized redox mediators can facilitate the electron transfer of such analytes like dopamine as shown in Figure 1.[3]

Different strategies for constructing CNTs based electrochemical sensors, the electrochemistry and electroanalytical chemistry of the CNTs are summarized and discussed, along with some relevant contributions in the development of electrochemical sensors based on CNTs. We describe the advantages of CNTs to promote different electron transfer reactions, in special those related to some important biomolecules. Some relevant applications of CNTs based electrochemical sensors to real sample analysis of some important biochemicals and some possible future trends are presented.[3,4]

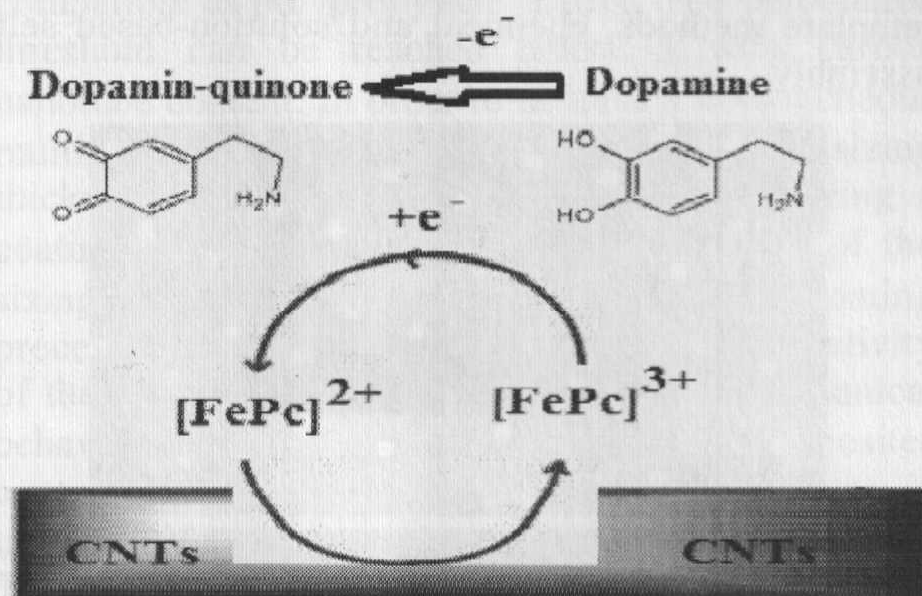


Fig. 1. Schematic representation of dopamine oxidation mediated by iron phthalocyanine immobilized on CNTs.

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## C12: Carbon Nanotube for Cardiovascular Engineering Applications

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During a heart attack, the heart's oxygen supply is cut off, and cardiomyocytes perish. Unfortunately, once these tissues are lost, they cannot be replaced and results in cardiovascular disease—one of the leading causes of death worldwide [1]. Recent understanding to what causes a myocardial infarction has lead to improved ways to combat such a deadly disease and improved health of patients with CVD. Unfortunately, the progression of CVD in the world is still growing [2]. For this reason, new methods to recognize and alleviate CVD in asymptomatic patients are necessary to inhibit the first symptoms of CVD from being the last.

Advancements in medical research have been targeted to understand and combat the death of these cardiomyocytes [2]. For example, new research (*in vitro*) has demonstrated that one can expand cardiomyocyte adhesion and proliferation using poly lactic-co-glycolic acid (PLGA) (50:50 (weight percent)) supplemented with carbon nanofibers (CNFs) to create a cardiovascular patch [3].

However, the examination of other cardiovascular cell types has not been investigated. Therefore, the purpose of this present *in vitro* study was to determine cell growth characteristics of three different important cardiovascular cell types (aortic endothelial, fibroblast and cardiomyocyte) onto the substrate. Cells were seeded onto different PLGA:CNF ratio composites to determine if CNF density has an effect on cell growth, both in static and electrically stimulated environments. During continuous electrical stimulation (rectangle, 2 nm, 5 V/cm, 1 Hz), cardiomyocyte cell density increased in comparison to its static counterparts after 24, 72 and 120 hours. A minor rise in Troponin I excretion in electrical stimulation compared to static conditions indicated nominal cardiomyocyte cell function during cell experiments. Endothelial and fibroblast cell growth experiments indicated the material hindered or stalled



proliferation during both static and electrical stimulation experiments, thus supporting the growth of cardiomyocytes onto the dead tissue zone. Furthermore, the results specified that CNF density did

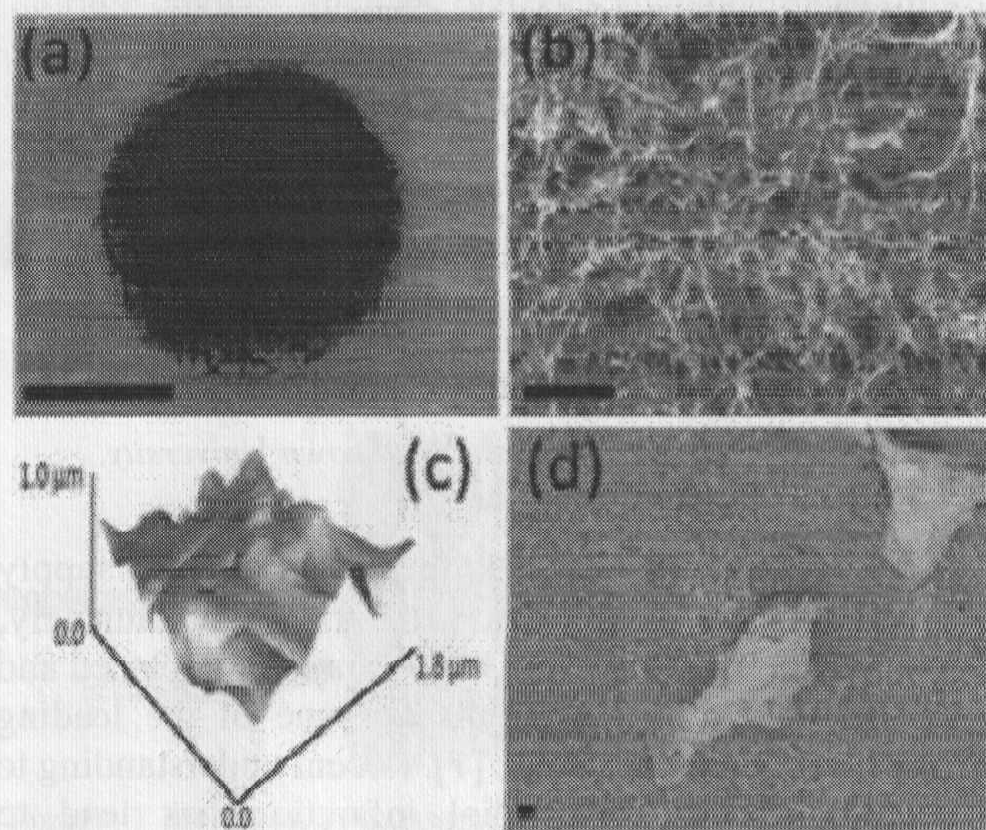


Fig. 1: a) A PLGA:CNF composite on a glass substrate for myocardial support (scale bar = 10 mm). b) Scanning electron micrograph of the PLGA:CNF composite at 10,000X (scale bar = 2  $\mu\text{m}$ ). Utilization of an atomic force microscope shows the addition of CNFs to the composite can increase surface nanometer sized characteristics and surface area (c). (d) A SEM image revealing specific cardiomyocyte morphological features on the PLGA:CNF (scale bar = 2  $\mu\text{m}$ ).

have an effect on PLGA:CNF composite cytocompatibility properties with the best results coming from the 50:50 [PLGA:CNF (weight percent:weight percent)] composite. Therefore, this study provides further evidence that a conductive scaffold using nanotechnology should be further research for various cardiovascular applications.

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### C13: Routes to carbon nanotube assembly and integration for applications

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Carbon nanotubes (CNTs), both single-walled (SWNTs) and multi-walled (MWNTs), have attractive physical properties for use in a range of fields, including electronics, photonics, energy and composite materials. [1] Precise control of the placement, orientation and/or structure of large numbers of CNTs is needed in order to optimize their performance for a given application. [2, 3]

Here, we review progress on carbon nanotube assembly and integration based on a variety of approaches and examine their use for different functional materials and devices. Controlled growth, along with pre- and post-growth approaches will be discussed, including catalyst patterning (Figure 1), template methods, chemical and solution-based self-assembly.

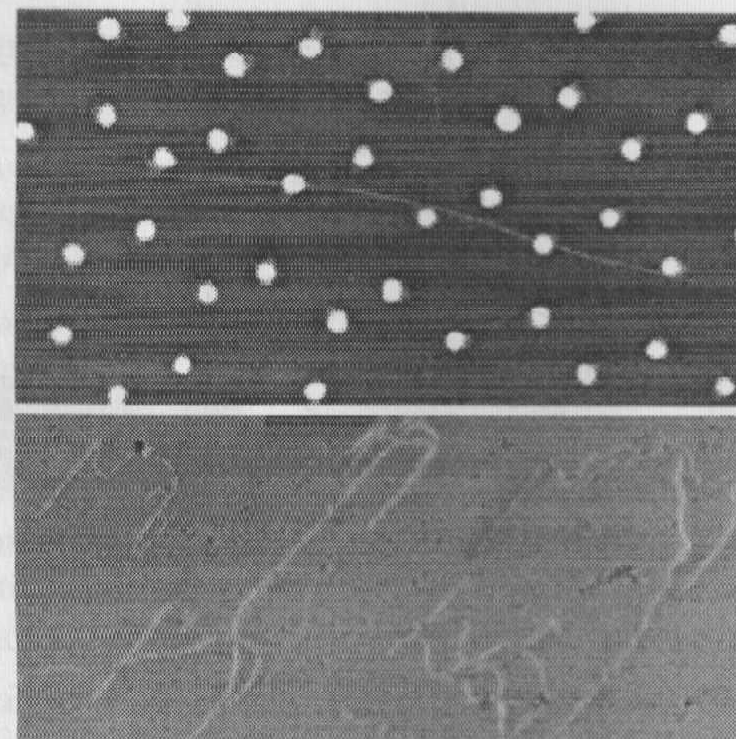


Fig1. Nanoscale breadboard patterning approaches [4, 5] for guiding SWNT growth: Left image shows carbon nanotube CVD growth from patterned catalyst particles; Right image displays CNT pattern formation on silicon dioxide guided by underlying nanoparticle breadboard.

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#### C14: Nanostructured Glass Fibers for Electro-Mechanical Response Sensor Applications in Glass Fiber Composites

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Carbon nanotube dispersions have been immersed in a maleated polypropylene film former system and applied to insulating glass filament yarns compatible to polypropylene matrix. The percolation threshold can be reached below 3 wt% carbon nanotube content. In order to achieve a homogeneous multifunctional interphase, the average sizing thickness must be above 450nm tailored during a coating process by varying the solid content of the sizing. The temperature and the velocity of the coating process have a great impact on the volume resistivity of the multifunctional interphase. Electro-mechanical behavior as sensors in unidirectional composites containing 50 vol% glass fiber reinforcement is monitored during tensile and compression loading. The largest electrical sensitivity is achieved for tensile loading in the axis of fibers.

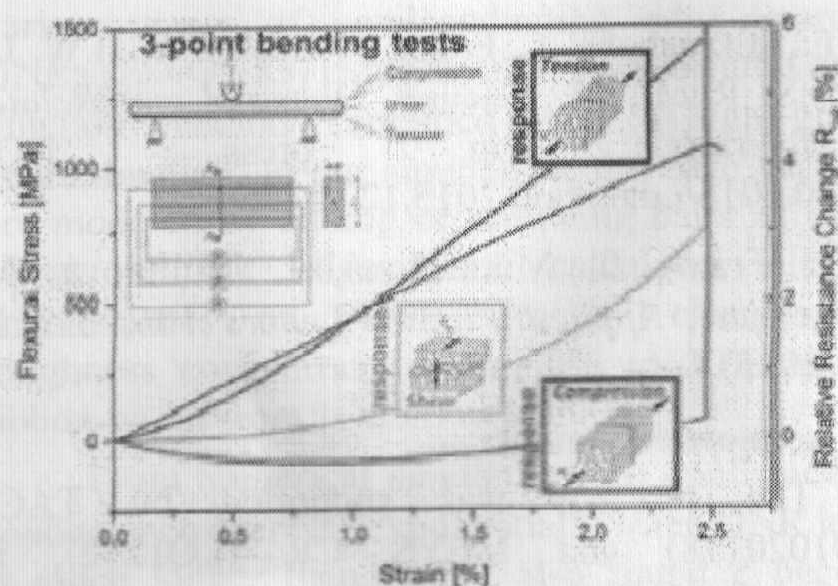


Fig1. The 3-point bending test demonstrated the potential for real time in-situ health monitoring during static loading. It is possible to distinguish between tensile, shear stresses or compression.

#### C15: Multiscale Patterning of Electrical Function in Graphene Oxide

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Oxygen-functionalized graphene, known as graphene oxide (GO), is a versatile two-dimensional material with highly tunable electrical, optical, and chemical properties. GO is easily deposited onto substrates from aqueous suspensions and can be converted from electrically insulating to conducting via reduction, which partially removes the oxygen from GO. Reduction is typically achieved through the use of highly toxic reagents or by using high temperatures in an inert atmosphere, conditions that are not amenable to large-scale manufacturing or to the selective patterning of conductive reduced-GO features in GO.

We have developed a simple voltage-based reduction process that operates under ambient conditions [1], and enables patterning of conductive features as small as 4 nm [2], the smallest achieved so far for reduced-GO. In this talk, we will present our latest work towards elucidating the electrical performance limits and mechanisms associated with voltage-induced reduction, and the prospects of using this approach for multiscale patterning. Preliminary results indicating electronic quantum confinement effects in nanoscale reduced-GO will be presented.

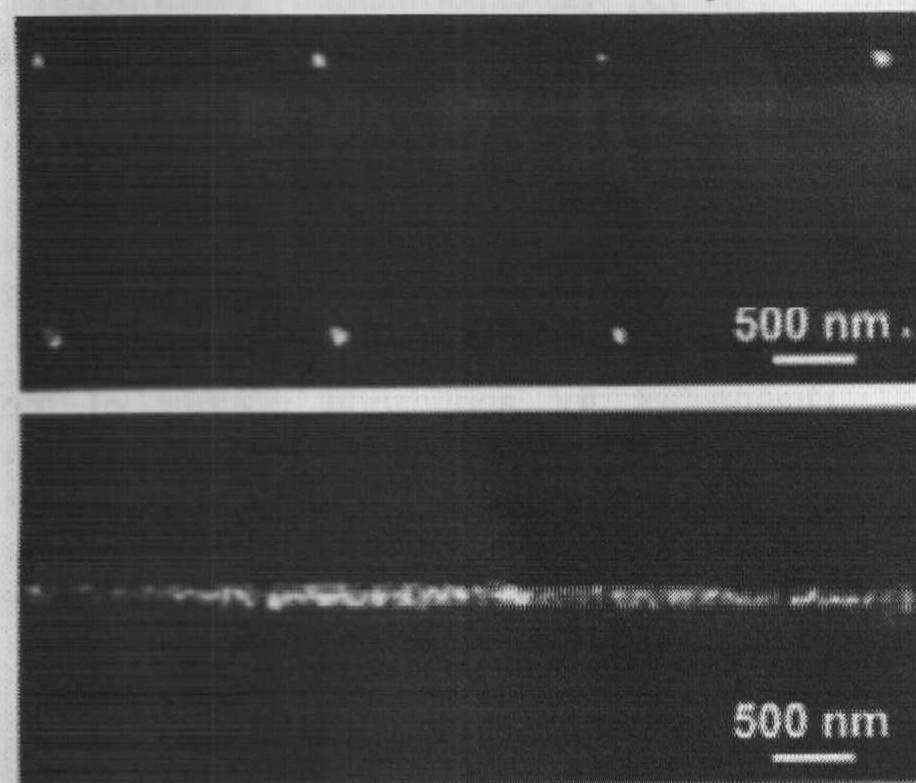


Fig1. Conductive reduced graphene oxide paths defined in insulating graphene oxide.

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2. C. Faucett, J. M. Mativetsky, *Carbon*, **95**, 1069 (2015).

### C16: Graphene examined with ultraslow electrons

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The reflection of very slow electrons from graphene on a substrate has been examined using a low-energy electron microscope (LEEM) [1,2]. In the LEEM, an arbitrarily low energy of primary beam electrons is secured with a high negative bias of the sample. The same principle has been applied to the scanning microscope [3] with the advantage of obtaining the transmitted electron image in addition to the reflected image [4]. With the exception of the parallel illuminating electron wave, the capabilities of the LEEM are preserved, and multiple imaging signals can be acquired simultaneously in the scanning SLEEM.

The LEEM examination revealed the graphene reflectivity fluctuating between 0 and 8 eV [1] and calculations confirmed the number of the reflectivity minima practicable to count the graphene layers [2]. The same has been found using SLEEM (Figure 1a,d) and even the predicted second band of fluctuations around 16 eV [5] was experimentally confirmed [6]. Non-supported free-standing graphene does not exhibit these reflectivity fluctuations (Figure 1b,e), though differences in transmissivity offer an alternative tool for counting the graphene layers [7] (Figure 1c,f). Moreover, the underlayer and overlayer mechanisms of growth of graphene on a substrate can be easily distinguished with the use of SLEEM [6].

Diagnostics for application practice of the number of possibly overlapped graphene flakes and, in particular, their uniformity and homogeneity can be successfully performed with SLEEM at high sensitivity and resolution, incomparable with, for example, Raman spectroscopy.[8]

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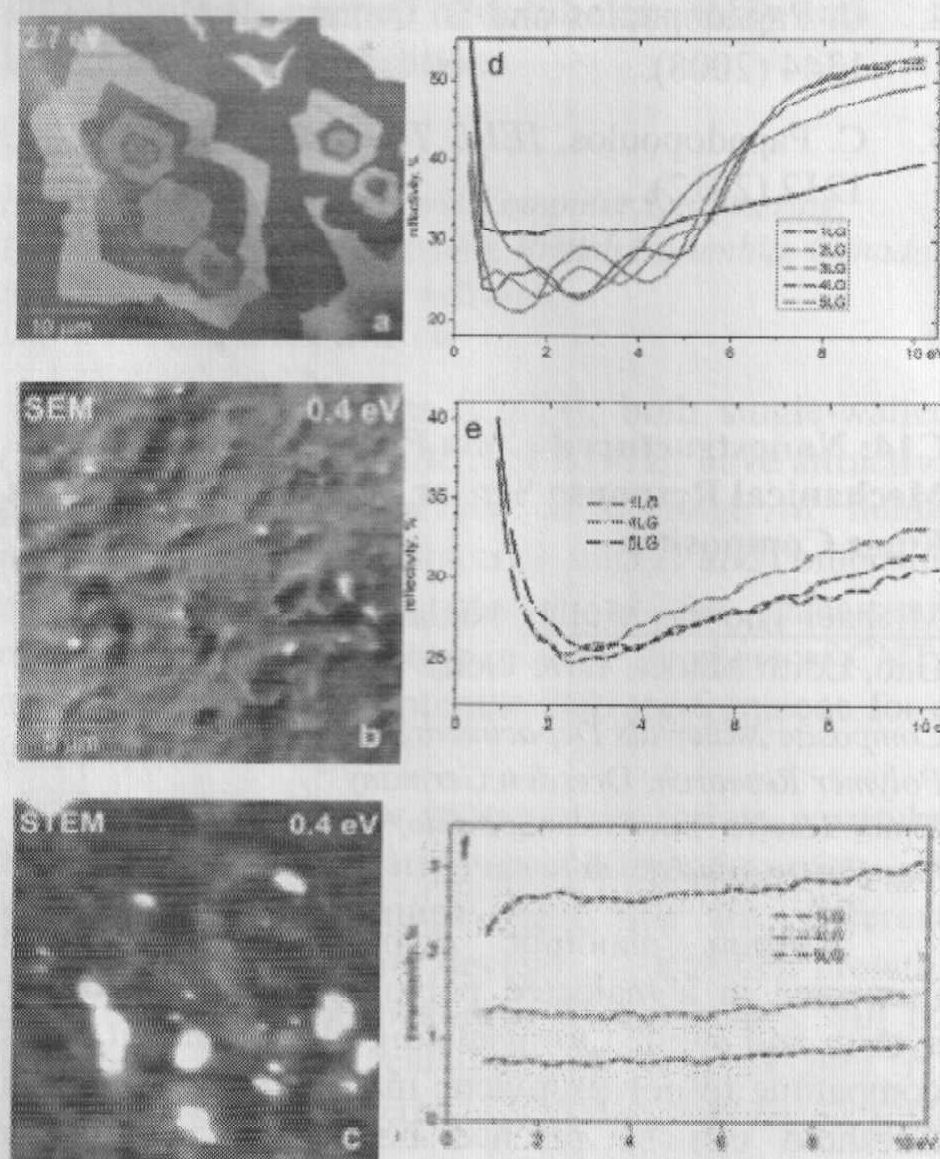


Fig. 1. SLEEM images of CVD graphene on Cu (a) and of free-standing graphene on lacey carbon in reflected (b) and transmitted (c) signals, reflectivity of supported (d) and free-standing (e) graphene and transmissivity of the later (f).

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### C17: Computational Design of Graphene-Nanoribbon Field Effect Transistors

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Graphene is expected to be a channel material of field effect transistors (FETs) because of its high carrier mobility. However, no band gap of the graphene is a serious problem for its FET application. One possible way to overcome the gap-opening problem is to process it in the form of a nanometer width ribbon, referred as graphene nanoribbons (GNRs). They have been successfully applied to FETs with high on-off ratio. A recent experiment reported that the resistance of GNRs increases exponentially with their length even at the room temperature [1]. This non-Ohmic behavior is due to the edge-vacancy of GNRs. The effects of edge-vacancy become more remarkable when the ribbon width becomes narrower in the future. There are many theoretical researches on electronic transport of edge-disordered GNRs (ED-GNRs) and these support the experimental result [2]. Recently, we investigated the conductance fluctuation of ED-GNRs and provided proof of such Anderson localization [3]. However, GNR-width and roughness concentration dependence are not clear yet.

In this study, the localization length  $\xi$ , characterizing the crossover between carrier localization and delocalization, was investigated for various types of semiconducting edge-disordered GNRs (ED-GNRs) using the non-equilibrium Green's function method combined with a tight-binding approximation. In our simulation, the edge vacancies are modeled by adding or removing pairs of carbon atoms at the edges. We calculated electrical conductances of ED-AGNRs by changing the roughness concentration from 0% to 30% and the ribbon-width from 1.48nm to 2.95nm.

From numerical simulation, we confirmed that conductance decrease exponentially when GNR length is much longer than  $\xi$ . We also found  $\xi$  becomes shorter when GNR width  $W$  is narrower and roughness concentration  $P$  is larger. Furthermore, we obtain an analytical formula of the localization length by the perturbation theory. It is determined that  $\xi$  is proportional to square  $W$  and inversely proportional to

$P$  as

$$\xi(\epsilon) = C \frac{W^2}{Pa_{cc}} \left( 1 - \frac{E_g^2}{4\epsilon^2} \right),$$

where  $C$  is a dimensionless coefficient,  $a_{cc}$  is carbon-carbon distance,  $E_g$  is electron bandgap and  $\epsilon$  is electron energy. This result provides important information for designing GNR-based FETs [4].

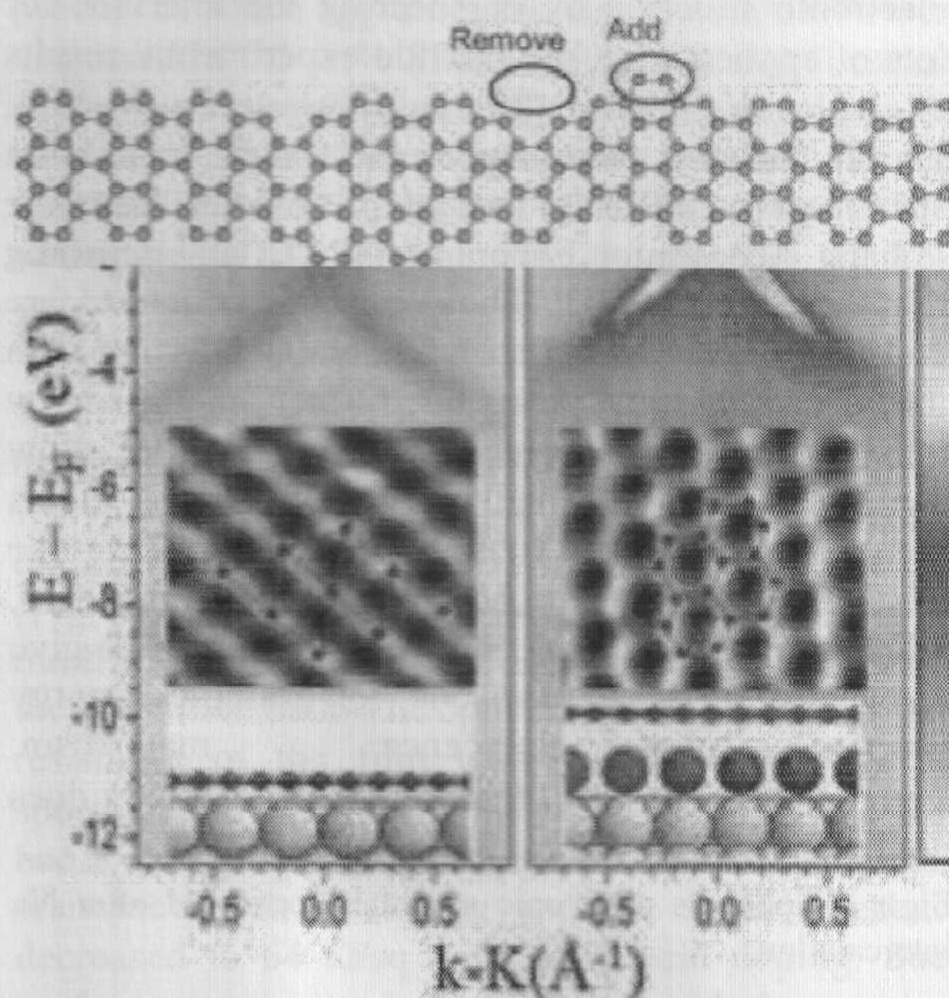


Fig.1: Schematic picture of edge-disordered graphene nanoribbon model

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### C18: Functionalizing graphene via interface engineering

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Graphene has many intriguing characteristics in its electronic structure. Its conduction and valence bands meet at a Dirac point and the energy depends linearly on the wave vector near the K-points, similar to a relativistic particle. However, real graphenes often show different electronic structures from the simple theoretical one depending on what they are facing. This means that it could be possible to tune graphene's electronic structure by engineering the interface for lots of applications. We provide experimental results of graphenes grown on different substrates, such as Cu, Fe, Ni, SiC, etc. using angle-resolved photoemission spectroscopy utilizing vacuum ultraviolet from the Pohang Accelerator Laboratory (PAL) and scanning tunneling microscopy. The electronic structures are considerably different depending on the interface with the substrates and can be further modified by intercalating or adsorbing foreign atoms. We show some data for the intercalation of several atoms between graphene and substrate together with the role of steps, defects, domain boundaries in real graphenes. Such an interface engineering could be useful to give a special function to graphene, for examples, energy gap, photoluminescence, magnetism, superconductivity, etc., that graphene originally does not have.

Fig1. Graphene's electronic structure recovered after Na intercalation

1. Young S. Park, Jae H. Park, Han N. Hwang, Tomba Singh Laishram, Kwang S. Kim, Myung H. Kang, and Chan C. Hwang, Quasi-free Standing Graphene Monolayer on a Ni Crystal through Spontaneous Na Intercalation, *Phys. Rev. X* **4**, 031016 (2014).
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#### P01: Studies on the equivalent serial resistance of carbon supercapacitor

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Equivalent serial resistance (ESR) is a crucial factor to effect on the density of power and energy for supercapacitor. In this work, we studied the influence of internal and external factors, including mechanical pressure, temperature, electrolyte concentration and loaded voltage on the performance parameters, especially on the ESR and capacitance for carbon supercapacitor. The results indicate that the ESR is mainly contributed from the interface between electrolyte and electrode. In addition, we found that the ESR can be significantly lowered by mechanical pressures and in consequence, the performance of supercapacitor can be improved dramatically for both power and energy density. Basing on the model of interface with a diffusion layer, we put forward a reasonable explanation for the variation of ESR and capacitance with the four factors of pressure, temperature, electrolyte concentration and loaded voltage.

#### P02: Partial Phase Coherence in Noise-Like Pulses Generated in Mode-Locked Laser Systems

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Fiber-based, passively mode-locked (ML) laser systems have become important instruments for a range of engineering and scientific applications due to their versatility and compactness. Among the ML mechanisms used in these devices, carbon nanotubes (CNTs) and graphene-based saturable absorbers have received a lot of attention, since they can be relatively easily fabricated and integrated with optical fibers [1, 2]. An interesting feature of these systems is that they cannot only generate stable coherent pulses such as solitons, Gaussian pulses, dissipative solitons, etc., but also, more complex pulse-dynamics such as noise-like



pulses (NLPs) [3]. NLP regimes are often characterized by the generation of noise-like femtosecond pulses bunched in wave packets traveling at a fundamental or higher harmonic cavity repetition rate. In the spectral domain, NLPs form highly structured broad spectra which fluctuate from pulse to pulse [3]. Therefore, a lack of phase coherence between successive NLPs is expected in this regime as shown in Ref. [3]. Nevertheless, with a similar cavity configuration as shown in Ref. [3], our group observed spectral interference patterns for successive NLPs [4]. We measured a fringe visibility  $V \sim 0.4$  across the central part of the NLP spectrum, indicating a pulse-to-pulse partial degree of coherence. Here, we present our recent studies carried out in our group to understand in more detail the partial degree of coherence observed in NLP regimes. At the conference we will discuss in more detail these specific features and discuss the possibility of the existence of a symbiotic regime in which stable pulses providing a certain degree of pulse-to-pulse coherence can interact with stochastic pulses continuously evolving in a laser cavity.

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### P03: Continuous dispersion of carbon nanotubes with minimal loss and damage

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Carbon nanotubes (CNTs) are an attractive candidate material for electronic devices owing to their excellent electronic properties, stability in ambient, flexibility, and compatibility with printing processes. Their uniform films with excellent conductivities have been realized by mild dispersion, centrifugation and printing process, however significant fractions of expensive CNTs are wasted during centrifugation. It is

important to establish efficient and simple process converting as-grown CNT powders into printed patterns with preserved quality for CNT-printed electronics.

In this work, we investigated continuous dispersion process of CNTs with minimal shortening of and damage to CNTs. It is the key to extract dispersed CNTs from the dispersion bath before being damaged while keeping undispersed CNT agglomerates in the bath to achieve high quality and yield of CNT dispersions [1]. We worked on a semi-continuous process in which agglomerated single-wall CNTs were dispersed in 0.5 wt% SDBS (sodium dodecylbenzene sulfonate) aqueous solution by tip-sonicator while the dispersed CNTs were continuously flow out through the metal mesh at the bottom of the bath by gradually adding the SDBS solution from the top (Fig. 1). This semi-continuous process yielded a CNT dispersion with very few CNT agglomerates (Fig. 2).

Then the dispersed CNTs were collected on a membrane filter via vacuum filtration and the CNT film was transferred to a PET film. The CNT film showed a uniform gray color with a few small CNT agglomerates (Fig. 3). Dispersion will be improved by adjusting the mesh pore size and the residence time of the solution in the sonication bath. The optical transmittance and sheet resistance of the film were measured by UV-Vis spectroscopy and four-point probe method. The film had a 78.4% optical transmittance and 99  $\Omega/\text{sq}$  sheet resistance without doping and the sheet resistance decreased to 64  $\Omega/\text{sq}$  with nitric acid doping. Such performance is very high compared with the solution-based CNT films in the previous reports and comparable with our recent report by a careful batch process with short-sonication of 3 min and centrifugation [1] (Fig. 4).

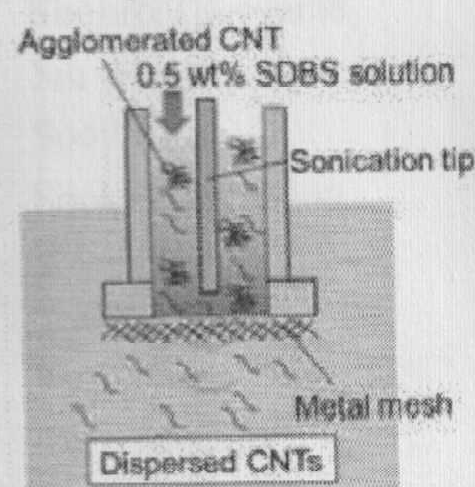


Fig. 1. Schematic of the semi-continuous sonication process

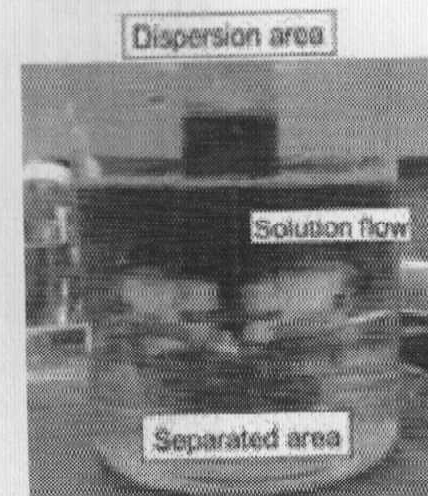


Fig 2. Digital image of the semi-continuous sonication process.



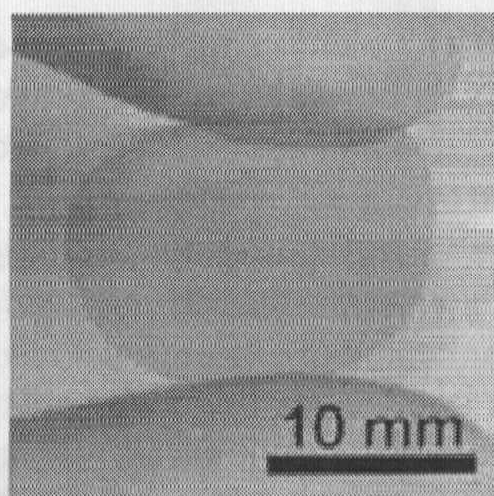


Fig. 3. A digital image of a typical transparent conductive CNT film on PET.

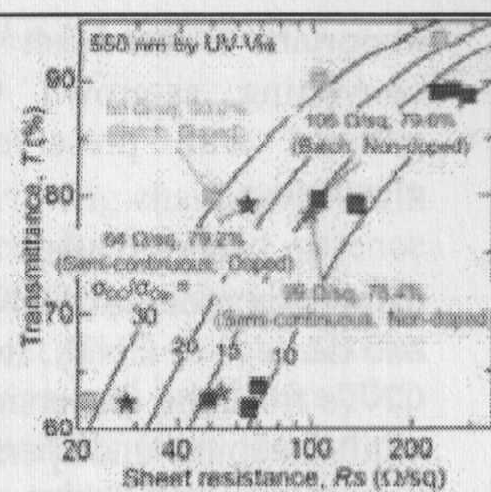


Fig. 4. Transparent conductive properties of the films by batch and semi-continuous processes.

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**B32: The Long and Winding Road Towards Single-Walled Carbon Nanotube Industrialization**

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After two decades of extensive research, single-walled carbon nanotubes (SWNT) are going to be industrialized at last. By the time of the conference, Nippon-Zeon will have announced that they will launch the first commercial SWNT production plant based on the super-growth technology in 2015. Concurrently, a couple of applications such as SWNT super-capacitors and composites would hit the market. To realize this, not only the development of mass production technique was necessary but also new concepts in CNT dispersion were crucial to keep the length of the long SWNTs and development of new application were required. Indeed, I envision that the “first” SWNT industrial applications are going to be very different from what we researchers had thought CNT would be useful for. In this talk I will present milestones, new concepts, new directions and aspects in synthesis, dispersion and applications of long SWNTs that have led to industrialization.



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## Innovative thinking and a global outlook: A school for life

The University of Electronic Science and Technology of China (UESTC) is located in Chengdu, the economic, cultural and transportation centre of West China. Chengdu is known as 'the land of abundance' and the 'hometown of the giant panda'. UESTC established the Institute of Fundamental and Frontier Sciences (IFFS) in 2014 specifically to attract experts in the areas of fundamental research, implement its vision for a high-level, research-focused university, strengthen its innovative capability, and enhance its academic impact. IFFS pursues intelligence, focus, freedom and success with a constant goal of advancing the promise of quantum physics at the nanoscale for processing and communicating electronic and photonic information to realize new knowledge and positively impact society.

### Why did you choose IFFS at UESTC?



"Launching the IFFS was a great accomplishment for the university and certainly a reflection of having the right people in the right place at the right time. It has been

an honour to lead this initiative. Guided by the university's three core strategies, we expect to attract more talented research-ers from around the world to become full-time and adjunct professors here and to advance both multidisciplinary and interdisciplinary collaborative research. Having the IFFS in Chengdu certainly adds another dimension to life — it's more than a job!"

**Prof. Zhiming Wang (Global Expert of the 1000 Talent Program) — Materials physics**



"I chose IFFS-UESTC because it (together with the Chinese government) offered me a generous start-up and support that I could never find at a

US university as a young scientist. The newly formed IFFS is young and vibrant and full of opportunity. I enjoy pursuing my research with great freedom and in an atmosphere of international collaboration. Moreover, Bib Gourmand-like restaurants are everywhere in Chengdu."

**Prof. Yijing Kang (1000 Global Talent Youth Expert) — Alternative energy**



"I chose to be part of IFFS at UESTC because of the Institute's vision and its focus on fundamental science. I enjoy my visits to IFFS in the beautiful city of Chengdu,

not just because of its nature and pandas, but also because of the opportunity to interact with bright young people who have high aspirations and are willing to work hard to achieve their dreams and goals. The leadership of UESTC has shown its vision and ambition in creating IFFS and I congratulate them."

**Prof. Chennupati Jagadish (Short-term Foreign 1000 Talents Program Expert, IFFS-UESTC & the Australian National University)**



"I was honoured to join IFFS because of the collaborative nature of this effort and the emphasis on basic research. IFFS is located in a uniquely

beautiful region of China and the Changjiang Chair Professorship is an opportunity to create a virtual bridge between Chengdu

and Montreal, to jointly train young scientists on projects of common interest. Last, but not least, I am linked to the IFFS members through both professional and personal ties, which makes the environment more friendly and the experience more rewarding."

**Prof. Federico Rosei (Yangtze River Scholar, IFFS-UESTC & INRS)**



"The UESTC has enjoyed a good reputation for innovation since it was founded in 1956. And the IFFS is a brand-new comprehensive re-

search institute focusing on fundamental and frontier research. It offers researchers a very free and cooperative research atmosphere. I enjoy pursuing a research career here very much. Besides that, Chengdu is a strategic location in China and the government is firmly committed to investing in research at Chengdu. This city is becoming an emerging hub for international research and is attracting world-class researchers."

**Prof. Xu Deng (1000 Global Talent Youth Expert) — Surface science**

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